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THE ANALYSIS OF TRACE IMPURITIES IN URANIUM COMPOUNDS USING SPARK-SOURCE MASS SPECTROMETRY

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THE ANALYSIS OF TRACE IMPURITIES IN URANIUM COMPOUNDS USING SPARK-SOURCE MASS SPECTROMETRY

by

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ATOMIC ENERGY CORPORATION OF SOUTH AFRICA, LIMITED

PRETORIA

CHAPTER FIVE

QUANTITATIVE ANALYSIS

5.1 *Calculation Methods*

The calculation method used to derive the formula for determination of relative sensitivity factors (RSF's) for impurity elements in different matrices relative to an internal standard is discussed in detail on page 138.

For clarity, the essential formulae are also given here:

$$\frac{Q_x}{Q_y} = \frac{K_x}{K_y} \cdot \frac{C_y}{C_x} \qquad \ldots\ldots\ldots\ldots\ldots \; (1)$$

where:

K_x/K_y is the RSF for element X relative to the internal standard, Y (see page 28).

Equation (1) can be rewritten as follows:

$$C_x = C_y \cdot \frac{\dfrac{K_x}{K_y}}{\dfrac{Q_x}{Q_y}} \qquad \ldots\ldots\ldots\ldots\ldots \; (2)$$

where:

C_x is the unknown concentration of an element X,
C_y is the known concentration of the internal standard,

Q_x/Q_y is the ratio between the exposure values of an element X and the internal standard at 50% transmission, and

K_x/K_y is the relative sensitivity factor for element X relative to the internal standard, which is derived from calibration plots as the slope of the regression line.

Equation (1) can be used to determine the RSF of any element X relative to any internal standard (IS) in any matrix Z. Rewriting equation (1) into the above notation gives:

$$(RSF^{X}_{IS})_Z = \left[\frac{\dfrac{Q_X}{Q_{IS}}}{\dfrac{C_{IS}}{C_X}} \right]_Z \quad \text{.........(3)}$$

This formula is directly related to the general formula for a RSF, namely:

$$RSF = \frac{C_{ms}}{C_{true}} \quad \text{.........(4)}$$

where:

C_{ms} is the concentration of an element X relative to an internal standard determined experimentally with the mass spectrometer, and

C_{true} is the true concentration of an element X relative to an internal standard where both concentrations are known.

The calculation method used to derive the formula which is used to determine the unknown background concentration of an element X in different matrices, Z, using different standards is given below. The general spark-source mass spectrometry equation applies:

$$(C_X)_Z = \frac{K_X}{(Q_X)_Z} \qquad \text{.........(5)}$$

where:

$(C_X)_Z$ is the unknown concentration of element X in matrix Z,
K_X is a constant for element X, and
$(Q_X)_Z$ is the instrument signal for element X in matrix Z.

Equation (5) also applies when a known standard (STD) is added to the matrix Z:

$$(C_X)_{Z+std} = \frac{K_X}{(Q_X)_{Z+std}} \qquad \text{.........(6)}$$

where:

$(C_X)_{Z+std}$ is the unknown concentration of element X in the matrix Z plus the known concentration of element X in the standard,
K_X is a constant (see equation (5)), and
$(Q_X)_{Z+std}$ is the combined instrument signal for element X and the standard in the matrix Z.

In order to determine the unknown background concentration $(C_X)_Z$ of element X in matrix Z, equations (5) and (6) are combined as follows:

$$(C_X)_{Z+std} - (C_X)_Z = K_X \left[\frac{1}{(Q_X)_{Z+std}} - \frac{1}{(Q_X)_Z} \right]$$

This difference is equal to the concentration of the added standard, expressed as $(C_X)_{std}$:

$$(C_X)_{std} = K_X \left[\frac{(Q_X)_Z - (Q_X)_{Z+std}}{(Q_X)_{Z+std} \cdot (Q_X)_Z} \right] \qquad \text{.........(7)}$$

$(Q_X)_Z$ and $(Q_X)_{Z+std}$ values can be determined as outlined on page 105 below.

$(C_X)_{std}$ values are known and K_X can be calculated. Inserting the K_X value for element X in equation (5) enables the determination of $(C_X)_Z$. This leads to the following equation:

$$(C_X)_Z = (C_X)_{std} \cdot \frac{(Q_X)_{Z+std}}{(Q_X)_Z - (Q_X)_{Z+std}} \qquad \text{.........(8)}$$

Equation (8) is the fundamental formula used to determine the background concentration of an element X in a matrix Z, using known prepared graphite standards. This formula will be used to determine background concentrations of impurity elements in U_3O_8 and UF_4 matrices in the following sections. The instrument signals of element X in both the matrix Z and the combination of matrix plus standard can be expressed relative to an internal reference standard (IS) (see page 28). Q_{IS} values are the same in the Z and Z+STD matrices for a particular choice of Y concentration.

Equation (8) then converts to:

$$(C_X)_Z = (C_X)_{std} \cdot \frac{(Q_X/Q_{IS})_{Z+std}}{(Q_X/Q_{IS})_Z - (Q_X/Q_{IS})_{Z+std}} \qquad \text{.........(9)}$$

This formula only holds true when $(Q_x/Q_{IS})_z$ is larger than $(Q_x/Q_{IS})_{z+std}$. The opposite can never happen in spark-source mass spectrometry because the concentration is inversely proportional to the instrument signal. Thus, the higher the concentration, i.e. when the standard is added to the matrix Z, the resultant instrument signal will be smaller than that for only the matrix Z.

5.2 *U_3O_8/graphite matrix quantitation*

5.2.1 *Blank correction*

In order to determine relative sensitivity factors (RSF's) for impurity elements in a U_3O_8/graphite matrix, the blank U_3O_8 sample must first be quantified. Considerable effort was initiated to obtain a blank U_3O_8 sample with few impurity elements to ensure a background spectrum relatively free from spectral lines. This blank base U_3O_8 sample (ES 0) was then mixed with a graphite powder, spiked with Y as an internal reference standard, in the ratio of five parts U_3O_8 to one part graphite by mass. The choice of this ratio has been discussed on page 30. The sample was then analysed several times to obtain an instrument signal, $(Q_x/Q_{\bar{y}})_{U_3O_8}$ for element X relative to the internal standard, Y, in a U_3O_8/graphite matrix. The exposure value for Y, $Q_{\bar{y}}$, is the mean of the singly and doubly charged species. The blank base U_3O_8 sample used for this purpose is stoichiometric i.e. 100 per cent U_3O_8.

To be able to quantify the impurity elements present in the blank base U_3O_8 sample, a range of graphite standards were prepared which contained the impurity elements under investigation in different concentrations, together with Y as internal reference standard. The method followed to prepare these graphite standards has been described on page 26. UCAR SP1 graphite powder was used for these standards. The concentration range of the standards is as follows:

U_3O_8 used: stoichiometric i.e. 84,8 per cent U.
Concentrations: 4 µg X /gC
20 µg X /gC
40 µg X /gC
100 µg X /gC
200 µg X /gC

Expressed relative to U, the concentrations $(C_x)_{std}$ for each impurity element X, become:

1 µg X /gU
5 µg X /gU
10 µg X /gU
25 µg X /gU
50 µg X /gU

The concentration of Y added to each of the above graphite standards as internal standard is 20 µg Y/gC or 5 µg Y/gU.

In addition to the above range of graphite standards using UCAR SP1 graphite, a range of check standards were also prepared using Ultra 'F' graphite. The main reason for preparing these check standards was to see whether results obtained for certain elements using UCAR SP1 graphite could not be improved by using Ultra 'F' graphite. The difference between these two graphite powders' background spectra for certain elements was used to check the results obtained from the UCAR SP1 range of graphite standards. This was especially useful for Fe, which has a high background concentration in UCAR SP1 compared to Ultra 'F'. Additional impurity elements not incorporated in the UCAR SPI graphite standards were now added to these check standards using Ultra 'F' graphite. These elements could not be added to the UCAR SP1 graphite because of spectral line interferences from elements already added. However due to the absence of these interfering elements in Ultra 'F' graphite these additional impurity elements could be added and analysed without any interference. Elements falling into this category were Li, W, P, Na, K and S. This fact also accounts for the low value for the number of analyses in Table 5.2 (see page 111) where the calibration curve parameters are listed.

The concentration range of these check graphite standards is as follows:

Concentrations: 20 µg X /gC
40 µg X /gC
80 µg X /gC
200 µg X /gC

Expressed relative to U, the concentration, $(C_x)_{std}$, becomes:

5 µg X /gU
10 µg X /gU
20 µg X /gU
50 µg X /gU

The concentration of Y added to each of the above graphite check standards as internal standard is 80 µgY/gC or 20 µgY/gU.

Using standard addition methods, each of the above graphite standards are mixed with the blank base U_3O_8 sample in the ratio of five parts U_3O_8 to one part graphite by mass. Similarly, as for the blank base U_3O_8/graphite matrix sample, each sample is analysed several times to obtain an instrument signal, $(Q_x/Q_y)_{U_3O_8+std}$, for element X relative to the internal standard in the blank base U_3O_8 plus the graphite standard. These instrument signals are used in equation (9) to calculate the concentration of element X in the blank base U_3O_8, $(C_x)_{U_3O_8}$

$$(C_x)_{U_3O_8} = (C_x)_{std} \quad \frac{(Q_x/Q_y)_{U_3O_8+std}}{(Q_x/Q_y)_{U_3O_8} - (Q_x/Q_y)_{U_3O_8+std}}$$

The results obtained to quantify the impurity elements in the blank base U_3O_8 sample are given in Table 5.1 as C_x(SSMS) in µgX /gU.

The concentration values for Na (20,9), Mg (26,0), Si (18,3) and Fe (20,3) are all very high in comparison to the concentrations of the graphite standards e.g. the 1, 5, 10 and 25 µgX/gU standards. This fact greatly influences the gradient of the calibration line. This is shown as follows:

On the x-axis of the calibration curve, the ratio C_y/C_x is plotted where $C_x = (C_x)_{std} + (C_x)_{U_3O_8}$. Thus when $(C_x)_{U_3O}$ is large, the ratio C_y/C_x becomes smaller where C_y is taken as constant. This makes the gradient, m, of the regression line

Table 5.1: Blank Base U_3O_8 (ES 0) quantification

Element	Charge State(+)	n	Std Error at 95 % CL (%)	C_x (SSMS) (µg X /gU)	Certified conc (µg X /gU)
B	1	18	10,4	9,8	0,07
Na	1	5	42,1	20,9	5
Mg	2	12	31,2	26,0	0,5
Al	2	18	13,3	9,6	1
Si	2	16	33,6	18,3	17
P	1 & 2	12	18,4	3,5	-
Ca	2	35	16,1	6,0	2,2
K	1 & 2	6	25,2	5,6	4
Ti	1 & 2	14	12,6	0,42	0,3
V	1 & 2	38	18,0	0,38	0,31
Cr	1 & 2	45	10,0	5,3	2
Mn	1 & 2	34	12,6	0,35	0,14
Fe	1 & 2	22	9,7	20,3	13
Co	1 & 2	26	8,1	0,30	0,1
Ni	1	28	10,5	2,4	0,8
Cu	1 & 2	26	12,3	0,5	0,3
Zn	1	31	7,3	1,78	1,66
Zr	1 & 2	36	12,9	3,5	0,5
Mo	2	12	18,7	2,5	0,3
Sb	1	25	14,1	1,22	1,2
Li	1	3	19,3	0,19	0,21

inaccurate and limits the calibration range. In this way the RSF is influenced directly by a high background concentration. Even elements with lower background concentrations e.g. B (9,8) and Al (9,6) influence the Q-values of the lower graphite standards with concentrations of 1, 5 and 10 µgX/gU. The same can be said for Ca (6,0), K (5,6) and Cr (5,3) which influence the two lowest graphite standards with concentrations of 1 and 5 µgX/gU. The rest of the elements in Table 5.1 have background concentrations which do not influence the calculation of relative sensitivity factors significantly.

The C_x *values in Table 5.1 determined for impurity elements in the blank base* U_3O_8 *are only for the elements in their elemental state. The hydrogenated and oxygenated species of the elements have not been considered. When analysing unknown* U_3O_8 *samples with the spark-source mass spectrometer, it is assumed that the same degree of hydrogenation and oxygenation of elements in the sample takes place as with the* U_3O_8 *calibration standard samples. This assumption is reasonable if the unknown sample is also stoichiometric* U_3O_8 *and the sparking parameters used to generate ions are identical for the* U_3O_8 *sample as for the* U_3O_8 *calibration standard samples.*

The chemical composition of the impurity elements within the U_3O_8 *samples are also assumed to be similar to those in the* U_3O_8 *calibration standard samples. The plasma generated between the two electrodes in the ion source provides the equalising locality for such differences. In this plasma the chemical structures are atomised and ionised and recombination of species takes place.*

The high standard errors at 95% confidence level (CL) for Na (42,1%) and K (25,2%) can be ascribed to the small number of data points (n = 5 for Na and n = 6 for K). The fact that the concentration of Na in the blank base U_3O_8 sample is quite high (C_x = 20,9 µg Na/gU) also plays a direct role in the relatively high uncertainty.

Similarly, the high standard errors at 95% CL for Mg (31,2%) and Si (33,6%) can also be ascribed to the high concentrations of these two elements in the blank base U_3O_8 sample (C_x = 26,0 for Mg and C_x = 18,3 for Si). This explains why the $(C_x)_{U_3O_8}$ values for these two elements fluctuated over the concentration range of the graphite standards. This fluctuation can further be enhanced by the position on the photoplate where the spectral lines of Mg at m/e 12,5 and of Si at m/e 14,5 are influenced by background emulsion fogging due to the strong spectral line of the major component, ^{12}C at m/e 12. This interference directly affects the results obtained for Mg and Si and can lead to large standard errors.

For the remainder of the impurity elements in the blank base U_3O_8 sample, the standard errors at a 95% CL show typical values comparable to the precision of the method, namely approximately 20%. The large values of n for these elements also ensures the reliability of the lower $(C_x)_{U_3O_8}$ values over the concentration range of the graphite standards.

In Table 5.1 concentration values of impurities in the base U_3O_8 material obtained with the spark-source mass spectrometer are compared with values obtained using different analytical techniques (see certified concentration column). These techniques are described on page 158. The main reason for some of the differences is the fact that the C_x (SSMS) values include the concentration of that particular element present in the graphite powder used. In other words, the C_x (SSMS) value reported is a combination of the concentration of that particular element in the blank base U_3O_8 sample as well as the concentration of that particular element in the UCAR SP1 graphite or Ultra 'F' graphite used. In this way, the impurities in the graphite powder have been quantified and should be kept in mind when using these graphite powders for future analyses.

Differences can also be due to contamination picked up from a variety of sources. An important source of contamination, especially at trace level concentrations, is from ordinary dust in the laboratory environment [24]. Typical elements found in dust samples collected in the laboratory and analysed for impurities included such elements as B, Mg, Al, Si and Ca. It has also been shown that the Na from NaCl in human perspiration is a significant source of Na contamination. Another source of contamination is from the stainless steel tools which are used in the preparation of the electrodes. Possible impurity elements include Al, Cr, Fe, Ni, Zr and Mo. It is thus difficult at this stage to identify the exact sources of contamination and to quantify these impurities. Proposals to prevent or minimise such contamination are discussed in Chapter 7 on page 166.

5.2.2 Calibration Curves

Calibration curves are constructed according to equation (1) on page 98. Q_x/Q_y is plotted on the y-axis. The value of C_x in C_y/C_x is taken as the sum of the concentrations of an element X in the prepared graphite standard plus the value in the blank base U_3O_8. Expressed as symbols, $C_x = C_{std} + C_{U_3O_8}$ where $C_{U_3O_8}$ is obtained from Table 5.1 on page 106.

The slope, K_x/K_y, of the calibration curve is the relative sensitivity factor (RSF) of that particular impurity element X present in the matrix U_3O_8 relative to an internal standard, Y. Calibration curve parameters are listed in Table 5.2 . The parameters c, r and n are discussed below. The standard error, s_m, in the slope is expressed in the form of the confidence limits of the slope, α, at a 95% confidence level (CL). These two parameters are discussed on pages 115 and 148 in terms of the statistical significance of the results.

The values of the intercept on the y-axis (c) are, with only a few exceptions, relatively close to the origin (0;0). The value of c must be evaluated in perspective with the magnitude of the scale of the y-axis. Elements with high RSF's have large absolute values for c. Examples of such elements are K^{2+} ($c = -0,6448$) and Bi^{2+} ($c = -1,0788$). Furthermore, elements with large α's also tend to have large values for c. This follows from the uncertainty in the slope of the regression line. Elements classified into this category are Mo^{1+} and W^{2+}. The intercept on the y-axis is reflected in the correlation coefficient of the fit of data to a regression line. A bad fit suggests that there are unreliable data points which, when included, would affect the intercept on the y-axis. Elements falling into this category are Mo^{1+} and Ba^{1+}. The value of c is not of importance as it is not incorporated directly into any calculations regarding concentration or RSF's.

However, the value obtained for r is an indication of the fit of the data to the regression line. Ideally, r should be unity. The values of r obtained in Table 5.2 are generally quite good. The rather poor fits of data for Fe^{1+} ($r = 0,8529$), Ba^{1+} ($r = 0,8972$) and Mg^{2+} ($r = 0,9278$) are also apparent from the

Table 5.2: U_3O_8 Calibration curve parameters

Element	Charge State(+)	m (RSF)	α (%)	c	r	n
B	1	1,1468	4,6	-0,0122	0,9961	19
Na	1	0,2483	28,2	0,0016	0,9716	7
Mg	2	1,7725	19,3	-0,0898	0,9278	21
Al	2	1,2399	10,9	0,0083	0,9740	22
Si	2	1,2836	15,1	-0,0197	0,9273	32
P	1	0,2178	20,8	0,0121	0,9839	7
P	2	1,3978	37,8	0,0511	0,9649	6
Ca	2	0,3035	12,2	-0,0216	0,9317	44
K	1	0,1073	15,7	-0,0014	0,9883	8
K	2	18,3676	24,2	-0,6448	0,9910	5
Ti	1	0,2598	16,0	0,0004	0,9660	15
Ti	2	0,4684	5,3	-0,0061	0,9969	12
V	1	0,3025	2,4	0,0248	0,9955	24
V	2	0,5004	19,9	0,0489	0,9580	13
Cr	1	0,2408	9,9	0,0087	0,9622	36
Cr	2	0,7199	9,4	-0,0082	0,9847	18
Mn	1	0,1529	10,3	0,0357	0,9753	23
Mn	2	1,0094	17,8	0,0324	0,9660	13
Fe	1	0,2301	23,6	0,0041	0,8529	30
Fe	2	1,1867	13,1	-0,0039	0,9809	13
Co	1	0,2697	4,0	-0,0049	0,9957	25
Co	2	1,2153	12,9	0,0362	0,9836	12
Ni	1	0,2397	5,7	0,0099	0,9898	29
Cu	1	0,2987	7,3	0,0215	0,9840	28
Cu	2	3,9934	8,2	0,0669	0,9924	13
Zn	1	0,6078	7,4	0,0074	0,9857	25
Sr	1	0,4877	10,0	0,1405	0,9767	23
Sr	2	0,3316	11,7	0,0109	0,9848	13

Table 5.2: Continued

Element	Charge State(+)	m (RSF)	α (%)	c	r	n
Zr	1	1,3375	7,8	0,0501	0,9839	25
Zr	2	0,6769	8,9	-0,0154	0,9911	13
Nb	1	1,3581	8,5	0,0273	0,9814	25
Nb	2	0,9780	10,1	-0,0180	0,9886	13
Mo	1	2,8176	19,2	-0,3758	0,9249	22
Mo	2	1,4294	9,1	-0,0468	0,9907	13
Ru	1	2,8572	6,0	-0,0171	0,9927	20
Ru	2	5,1368	19,2	0,0095	0,9609	13
Cd	1	1,1031	13,2	0,1175	0,9702	25
In	1	0,5853	12,5	0,1331	0,9607	25
In	2	7,7360	11,9	0,0027	0,9842	13
Sb	1	1,7565	16,9	0,0113	0,9342	24
Sb	2	7,0408	7,5	-0,1386	0,9937	13
Ba	1	0,5416	23,0	0,6769	0,8972	22
Ba	2	0,4784	10,5	0,0230	0,9879	13
Sm	1	4,2008	45,0	0,0000	0,9310	7
Sm	2	0,6019	4,9	0,0437	0,9945	26
Eu	1	4,6455	6,2	0,0082	0,9962	12
Eu	2	0,6633	9,7	0,0179	0,9743	26
Gd	1	3,6455	7,4	-0,0127	0,9960	12
Gd	2	0,9391	5,5	-0,0087	0,9939	20
Dy	1	7,2053	6,3	-0,1353	0,9960	12
Dy	2	0,6998	5,5	0,0883	0,9922	24
W	2	2,1239	40,3	0,5395	0,9604	6
Bi	2	20,1841	14,8	-1,0788	0,9681	16
Th	2	2,0486	7,7	-0,0852	0,9889	19
Li	1	0,0243	7,1	0,0002	1,0000	5

large errors in the slopes where α for Fe^{1+} = 23,6%, α for Ba^{+} = 23,0% and α for Mg^{2+} = 19,3%. Another explanation for the poor calibration lines for Fe^{1+} and Mg^{2+} is the high values of these elements in the blank base U_3O_8, where $C_{U_3O_8}$ = 20,3 µg Fe/gU for Fe^{1+} and $C_{U_3O_8}$ = 26,0 µg Mg/gU for Mg^{2+}. This is in spite of the large number of data points (n) used to draw the calibration curves for these elements. The calibration graph for Fe^{1+} in a U_3O_8 matrix is given in Figure 5.1 as an example of a poor calibration curve.

Good calibration curves were obtained for Co^{1+} and V^{1+} as indicated by the correlation coefficients obtained for these elements where r = 0,9957 and r = 0,9955, respectively. Factors contributing to the good fit of data points for these elements is the fact that they both have very small α values where α = 4,0% for Co^{1+} and α = 2,4% for V^{1+}. Another reason is the fact that they both have small concentrations in the blank base U_3O_8 where $C_{U_3O_8}$ = 0,3 µgCo/gU for Co^{1+} and $C_{U_3O_8}$ = 0,38 µgV/gU for V^{1+}. In both cases the value of n is large where n = 25 for Co^{1+} and n = 24 for V^{1+}. A typical example of a good calibration curve is given in Figure 5.2 for Co^{1+} in a U_3O_8 matrix. Another good calibration curve is obtained for B^{1+} where the concentration obtained in the blank base U_3O_8 is fairly high where $C_{U_3O_8}$ = 9,8 µgB/gU for B^{1+}. The other parameters coupled to this calibration curve are: r = 0,9961; n = 19 and α = 4,6%. This calibration line is also given in Figure 5.3 as a good line where a large background concentration is present.

The value of n in Table 5.2 is the number of data points where each analysis was taken as a separate data point. The value for the blank is also incorporated in n as a data point.

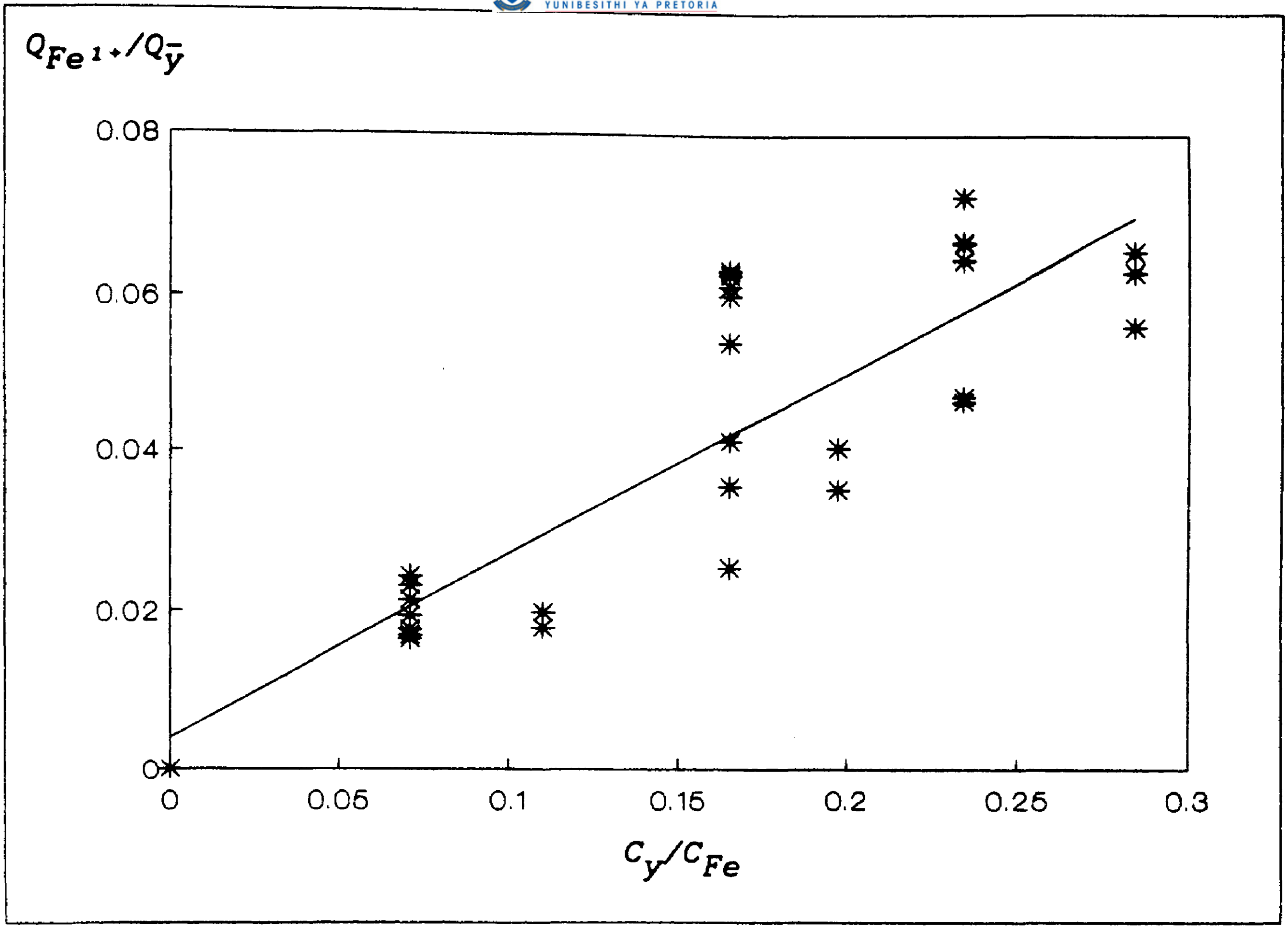


Figure 5.1: *Calibration curve for* Fe^{1+} *in a* U_3O_8*/graphite matrix*

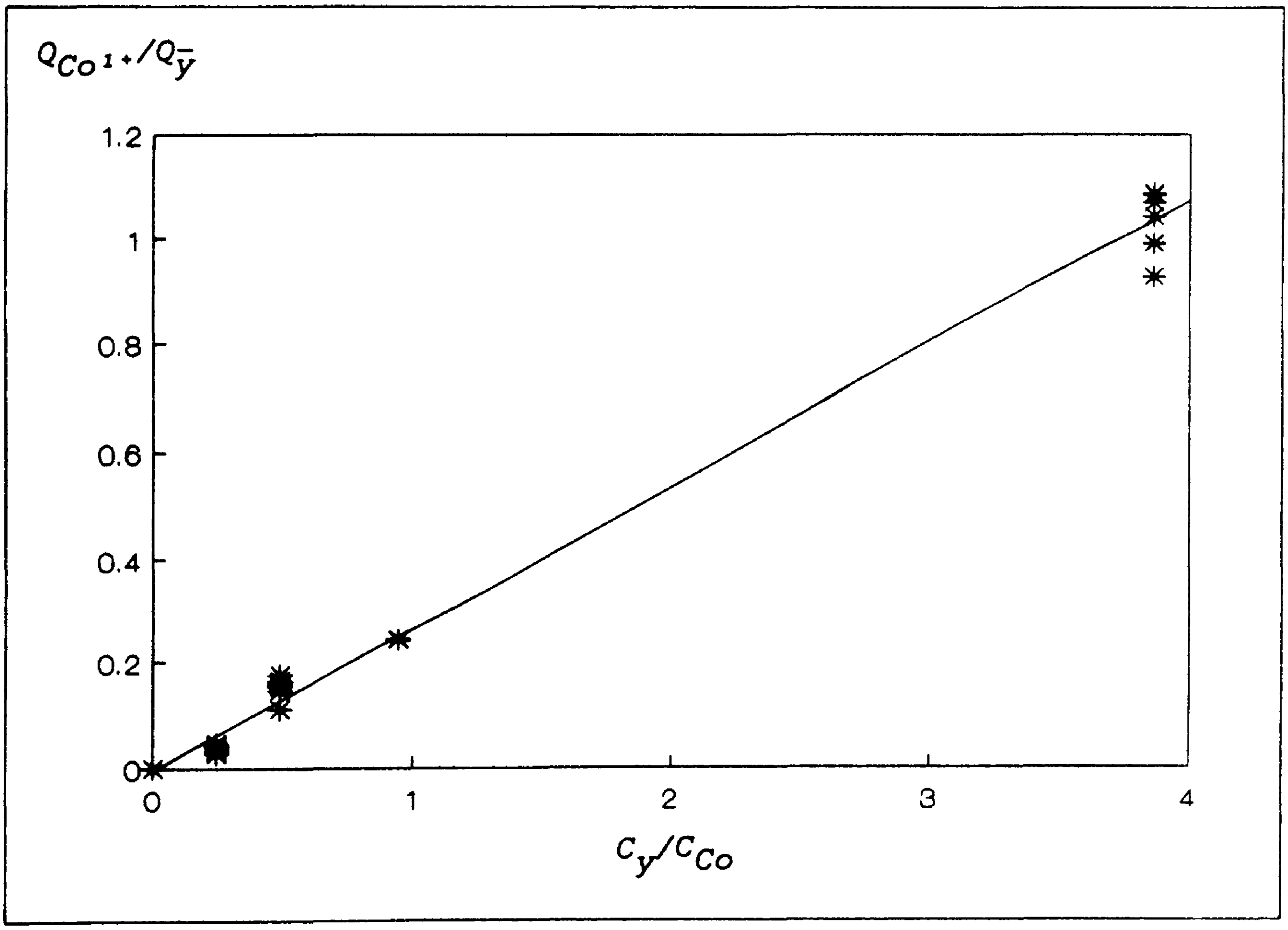


Figure 5.2: *Calibration curve for* Co^{1+} *in* U_3O_8*/graphite matrix*

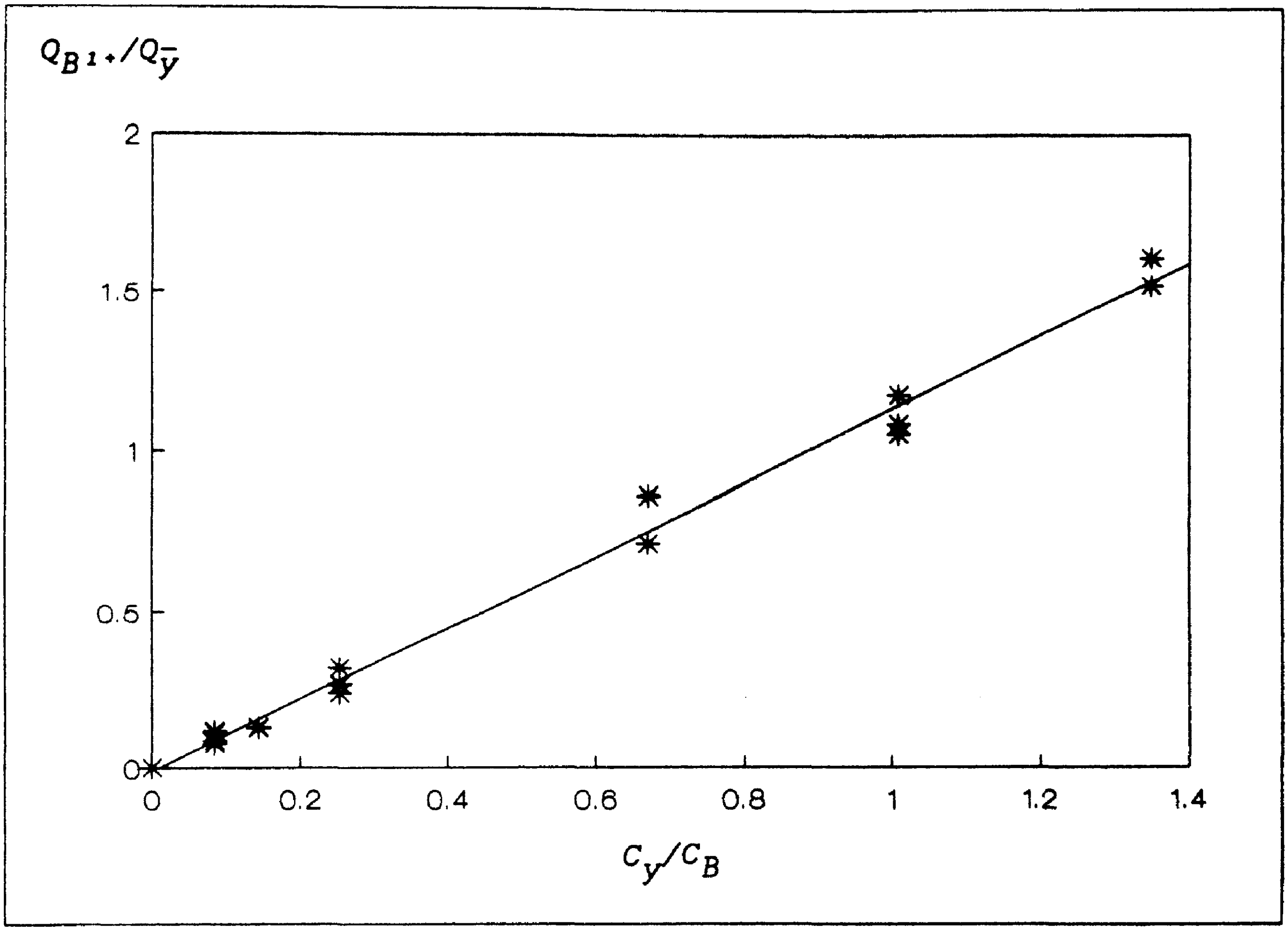


Figure 5.3: Calibration curve for B^{1+} in a U_3O_8/graphite matrix

5.2.3 Relative sensitivity factors (RSF's) - U_3O_8

The instrument sensitivity for a particular element is totally unique for a specific spark-source mass spectrometer and detection system. Different RSF's will be obtained for an element using a radio frequency (RF) spark compared to a triggered low-voltage discharge spark as was used in this investigation.

Another important factor to be considered is that a RSF for a particular element X will differ from matrix to matrix [25]. This is illustrated when comparing RSF's obtained for mutual elements (e.g. Al, P, Ca, Si and Zn) for both a UF_4 and a U_3O_8 matrix. Differences in this case could be ascribed, among other reasons, to the fact that in a UF_4 matrix, fluorination occurs within the plasma resulting in less elemental species of ions.

A RSF is also unique with regard to a particular internal reference standard.

It was beyond the scope of this investigation to determine whether a RSF for an element in a U_3O_8 matrix will differ from that for another uranium oxide matrix, for example UO_2 or UO_3. It is the author's opinion that there would not be a significant difference because the combinations of uranium and oxygen would create very similar plasma conditions [11]. In all uranium oxide matrices, there is an over-abundance of oxygen species generated within the plasma.

Correlations between physico-chemical properties of various elements as impurities and relative sensitivity factors have been published [23, 26]. Instead of using standards to determine RSF's, some authors have determined theoretical RSF's from making use of various combinations of physico-chemical properies of the elements. For the purpose of this investigation, an attempt will only be made to explain certain of the anomalies observed in the experimentally determined RSF's.

Physico-chemical properties such as heats of vaporisation, electrical resistivity, thermal conductivity, ionisation potentials, atomic radii and melting points were studied and some correlations drawn. These correlations are qualitative at their best. Due to the complexity of plasmas in relation to the physico-chemical properties, anomalies cannot be adequately explained in this qualitative fashion. It would require computer simulations involving chemical and physical studies in order to relate the properties to RSF's. This is a very complex task which has not been described in the literature and is beyond the scope of this thesis. Qualitative comments will nevertheless be offered for some of the observations.

The high relative sensitivity factors (RSF's) obtained for a few of the impurity elements in a U_3O_8/graphite matrix can be related to their physico-chemical properties with some degree of confidence. Elements which do not readily form ions of a particular species tend to have high RSF's for this species. A prime example is K^{2+} which has a very low ion yield for doubly charged species. A factor in this regard is the fact that potassium has only one valence electron in its outermost shell (4s orbital). This valence electron is readily lost to form the singly charged state having the noble gas structure of argon. Thereafter, it would require far more energy to remove a second electron to form the doubly charged species. This fact could be related to the second ionisation potential (I_P^{II}) for K which, together with the other alkali-earth metals, has the highest I_P^{II} of all the elements. The RSF of 18,3676 obtained for K^{2+} differs considerably from that obtained for K^+ (RSF = 0,1073). It is evident that K^+ ions are formed in great abundance in the mass spectrometer. Another element which has a small RSF is Li (RSF = 0,0243). Both Li and K are alkali-earth metals of group IA which readily lose an electron to have a noble gas structure. In the case of Li, this would be helium. Na also has a relatively small RSF namely 0,2483. All the group IA elements have of the lowest melting points which would contribute to the high yield of ions for these elements and the subsequent low RSF's. These elements also have of the lowest electrical resistivity of all the elements present. This fact could also contribute to these elements being atomised and ionised more easily.

Bismuth has a high electrical resistance which could account for the very poor ion yield for the Bi^{2+} ion and the subsequent high RSF value. Only the doubly charged Bi^{2+} was recorded (see page 71). Bismuth is also the most diamagnetic of all the metals and the thermal conductivity is lower than any metal, except for Hg. Both the electrical resistivity and the thermal conductivity are physico-chemical properties which play a role in the generation of the plasma between the two electrodes in the ion-source.

Another group of elements having relatively high RSF's are the singly charged species of the rare-earth metals e.g. Sm, Eu, Gd and Dy. These all have relatively high electrical resistivities and large atomic radii. It was found that the ion yield for doubly charged species was greater than for the singly charged species. This can be demonstrated by plotting the number of ions yielded against the charge state [27].

It would seem that the larger the atom becomes, the fewer ions reach the photoplate, probably due to their momentum and collisions in the flight tube. Elements falling into this category are W^{2+}, Th^{2+}, Sb^{2+}, In^{2+}, Ru^{2+}, Ru^{1+} and Mo^{1+}, and high RSF's could be expected. However, it should be taken into account that the number of ions generated in the ion source also plays a determining role.

The relatively high RSF for Cu^{2+} (RSF = 3,9934) is of interest as it is the highest of the 3d transition elements. Cu and Ag *have of the lowest electrical resistance as well as the highest thermal conductivity. They both are group IB elements having electron configurations such that their d-orbitals are filled and having one electron in the outermost s-orbital. The filled d-orbitals lead to stability and an electron is readily lost from the half filled s-orbital. In order to lose another electron to form* Cu^{2+} *species, more energy is required to remove an electron from a paired 3d orbital resulting in a high RSF for* Cu^{2+}.

Only a few of the physico-chemical properties of the elements have been referred to in order to explain some of the anomalies obtained with RSF's for impurities in a U_3O_8*/graphite matrix. Properties such as bond strengths in diatomic molecules and heats of formation of gaseous atoms from elements in their standard states should also be included when attempting to explain these anomalies.*

The RSF's obtained from calibration curves can be checked by making use of the instrument signals obtained. The ratio between the instrument signal for the singly charged state of an element and the instrument signal for the doubly charged state of the same element at a concentration level should be the same as the ratio between the RSF of the singly charged state of the particular element and the RSF for the doubly charged state of that element. The ratio X^{1+}/X^{2+} *is independent of the concentration of element X. A number of elements were measured both in the singly and doubly charged states at two different concentration levels. The means of the ratio* X^{1+}/X^{2+} *between these two concentrations were compared and good correlation was obtained. This ratio was used to test the ratio RSF* X^{1+}*/RSF* X^{2+} *for the same element using the RSF's obtained in Table 5.3. Good agreement was obtained for most of the elements, which confirmed that outliers did not seriously influence the determination of RSF's. The ratio* X^{1+}/X^{2+} *can be used with a RSF for* X^{1+} *to get an estimate of the RSF for* X^{2+} *and vice versa.*

Table 5.3: Relative Sensitivity Factors: U_3O_8/Graphite Matrix

RSF Singly charged Species	Element	RSF Doubly charged Species	$\frac{RSF\ X^{1+}}{RSF\ X^{2+}}$	X^{1+}/X^{2+} $C_x = 10 \mu g X/gU$	X^{1+}/X^{2+} $C_x = 50 \mu g X/gU$
0,0243	Li				
1,1468	B				
0,2483	Na				
	Mg	1,7725			
	Al	1,2399			
	Si	1,2836			
0,2178	P	1,3978			
	Ca	0,3035			
0,1073	K	18,3676			
0,2598	Ti	0,4684			
0,3025	V	0,5004	0,60	0,60	0,58
0,2408	Cr	0,7199	0,33	0,34	0,37
0,1529	Mn	1,0094	0,15	0,15	0,15
0,2301	Fe	1,1867	0,19	0,20	0,20
0,2697	Co	1,2153	0,22	0,22	0,21
0,2397	Ni				
0,2987	Cu	3,9934	0,07	0,08	0,09
0,6078	Zn				
0,4877	Sr	0,3316	1,47	1,55	1,85
1,3375	Zr	0,6769	1,98	2,03	2,06
1,3581	Nb	0,9780	1,39	1,42	1,27
2,8176	Mo	1,4294	1,97	2,02	2,02
2,8572	Ru	5,1368	0,56	1,37	0,67

Table 5.3: *Continued*

RSF Singly charged Species	Element	RSF Doubly charged Species	$\frac{RSF\ X^{1+}}{RSF\ X^{2+}}$	X^{1+}/X^{2+} C_x=10μgX/gU	X^{1+}/X^{2+} C_x=50μgX/gU
1,1031	Cd				
0,5853	In	7,7360	0,08	0,08	0,09
1,7565	Sb	7,0408	0,25	0,25	0,24
0,5416	Ba	0,4784	1,13	1,08	1,19
4,2008	Sm	0,6019	6,98	6,63	6,55
4,6455	Eu	0,6633	7,00	7,05	7,58
3,6455	Gd	0,9391	3,88	3,97	3,89
7,2053	Dy	0,6998	10,30	10,64	9,76
	W	2,1239			
	Bi	20,1841			
	Th	2,0486			

5.3 UF_4-graphite matrix quantitation

5.3.1 Blank correction

In order to determine relative sensitivity factors (RSF's) for impurity elements in a UF_4/*graphite matrix, the blank* UF_4 *sample which was to be used to simulate the matrix material first had to be quantified. Considerable effort was initiated to obtain a blank* UF_4 *sample with the least impurity elements to ensure a background spectrum relatively free from spectral lines. This blank* UF_4 *sample was mixed with graphite powder, spiked with Y as an internal reference standard, in the ratio of one to one by* mass. The sample was then analysed several times to obtain an instrument signal $(Q_x/Q_{\bar{y}})_{UF_4}$ for element X relative to the internal standard, Y. The exposure value for Y, $Q_{\bar{y}}$, is the mean for the singly and doubly charged species. The blank UF_4 sample used for this purpose is stoichiometric i.e. 100 per cent UF_4.

A range of graphite standards were prepared with the impurity elements of interest at different concentrations, together with Y as internal reference standard. The method followed to prepare these graphite standards is given on page 26. The concentration range of these graphite standards is as follows:

UF_4 used: stoichiometric i.e. 75,8% per cent U.
Concentrations: 100 µg X /g UF_4
200 µg X /g UF_4
500 µg X /g UF_4
700 µg X /g UF_4
1 000 µg X /g UF_4

Expressed relative to U, the concentrations $(C_x)_{std}$ for each impurity element X, become:
132 µg X /gU
264 µg X /gU
660 µg X /gU
924 µg X /gU
1 319 µg X /gU

The concentration of Y added to each of the above graphite standards as internal standard is 132 µgY/gU.

These standards were used to quantify the impurity elements in the blank UF_4. Using standard addition methods, each of the above graphite standards was mixed with the blank UF_4 sample in the ratio of one to one by mass. Similar to the blank UF_4 graphite matrix sample, each spiked sample is analysed several times to obtain an instrument signal, $(Q_x/Q_{\bar{y}})_{UF_4+std}$, for element X relative to the internal standard, Y. The concentration of each element X can be determined on the basis of equation (9) discussed on page 101:

$$(C_x)_{UF_4} = (C_x)_{std} \bullet \frac{(Q_x/Q_{\bar{y}})_{UF_4+std}}{(Q_x/Q_{\bar{y}})_{UF_4} - (Q_x/Q_{\bar{y}})_{UF_4+std}}$$

Results are given in Table 5.4 as C_x, in µgX/gU.

Table 5.4: Blank UF_4 quantification

Element	Isotope	Isotopic Abundance(%)	Charge State	n	Std Error at 95% CL (%)	C_x (µg X/gU)
Al	27	100	2	8	21,36	5,6
P	31	100	2	5	34,85	76,7
Ca	40 42	96,94 0,65	2 2	9	12,48	25,2
Si	30	3,09	1	5	13,59	77,4
S	32	95,0	1	5	38,74	385,4
Cl	35 37	75,72 24,28	1 1	10	21,35	52,5
Zn	64 67	48,89 27,77	1 1	8	23,78	4,0

The concentration value for S is quite high (385,4 µgS/gU). This greatly influences the calibration line. On the x-axis of the calibration curve, the ratio C_y/C_x is plotted where $C_x = (C_x)_{std} + (C_x)_{UF_4}$. When the background concentration of an element X in the blank UF_4, $(C_x)_{UF_4}$, is large, the ratio C_y/C_x becomes smaller, where C_y is taken as constant. This makes the gradient of the regression line inaccurate and limits the calibration range. The other impurity elements have background concentrations which do not influence the calibration.

The C_x values in Table 5.4 determined for impurity elements in the blank UF_4 are only for the elemental states. The fluorinated species of the elements have not been considered. When analysing UF_4 samples with the spark-source mass spectrometer, it can be assumed that the same degree of fluorination of the elements takes place in the sample as with the UF_4 calibration samples. This assumption is valid if the unknown sample is also stoichiometric UF_4 and the sparking parameters used to generate ions are identical for the UF_4 sample as for the UF_4 calibration samples.

The chemical structures of the impurity elements in the UF_4 sample are assumed to be similar to those in the UF_4 calibration samples. The plasma generated between the two electrodes in the ion source provides the equalising locality for such differences. In this plasma the chemical structures are broken in the process of atomisation and ionisation and recombination of species can take place.

The preparation and characterisation of graphite standards to obtain relative sensitivity factors (RSF's) for impurity elements in a UF_4 sample were done under serious production pressures due to the study of reactions in the uranium fuel production process and time was not allowed to analyse the blank UF_4 sample more comprehensively. It was nevertheless decided to include the results in this thesis as they were reasonable in terms of the precision of the method and made a major contribution to the solving of the production problems at the time. The fact that the UF_4 work was done as an additional project under severe time constraints must be kept in mind when accessing the small number of data points on which the principles have been demonstrated.

The high standard errors at 95 % confidence level (CL) for P (34,85 %) and S (38,74 %) can be ascribed to the small number of data points which were statistically acceptable. This shows how the $(C_x)_{UF_4}$ values for these two elements fluctuated over the concentration range of the standards resulting in the C_x values at higher concentrations being rejected leaving n = 5 with still a larger error in the remaining $(C_x)_{UF_4}$ values. The standard error at 95 % CL obtained for Si (13,59 %) with n = 5 seems to be the exception where the remaining $(C_x)_{UF_4}$ values show a better standard error at lower concentration levels of the graphite standards. For the above three elements, namely P, Si and S, their concentrations present in the UF_4 sample are the highest, which has a direct influence in the standard errors at 95 % CL.

For the remainder of the impurity elements in the blank UF_4 sample, the standard errors at a 95 % CL show typical values comparable to the precision of the method, namely ~ 20 %. The larger value of n for these elements also shows the reliability of the lower $(C_x)_{UF_4}$ values over the concentration range of the graphite standards.

5.3.2 Calibration curves

The procedure used to construct calibration curves is given in detail on page 137. A few interesting observations are highlighted below.

Similar to procedures followed for the U_3O_8 matrix (see page 109), the instrument signal, $Q_x/Q_{\bar{y}}$, is plotted on the y-axis and the ratio between the concentrations, C_y/C_x, is plotted on the x-axis. The value of C_x in C_y/C_x is taken as the sum of the concentrations of an element X in the prepared graphite standard plus the value of the blank UF_4, expressed as, $C_x = C_{std} + C_{UF_4}$, where C_{UF_4} is obtained from Table 5.4.

The slope of the resultant curve is the relative sensitivity factor (RSF) of that particular impurity element X present in the matrix UF_4 relative to an internal reference standard, Y.

Theoretically, the calibration curve should pass through the origin (see page 139). The values of the intercept on the y-axis, c, listed in Table 5.5 are in accordance with this fact for most of the elements. The values obtained for P and Cl must be kept in perspective as the values of m for these two elements are also large in magnitude compared to the rest. Negative values for c on the y-axis could indicate a minimum detection value for C_x on the x-axis. Below this minimum detection value, non-linearity is evident. For the purpose of this investigation, the highest concentration measured was 1319 μg X/gU. Al and Zn display good linearity over the entire concentration range.

Table 5.5: UF_4 Calibration curve parameters

Element	Isotope	Isotopic Abundance(%)	Charge State	m (RSF)	α (%)	c	r	n
Al	27	100	2	2,0059	0,84	0,0008	0,9999	10
P	31	100	2	25,7454	10,6	-0,9496	0,9917	10
Ca	40 42	96,94 0,65	2 2	0,6104	3,64	-0,0169	0,9980	16
Si	30	3,09	1	0,9438	8,38	-0,0490	0,9948	10
S	32	95,0	1	0,6891	26,9	-0,0123	0,9575	9
Cl	35 37	75,72 24,28	1 1	20,0095	4,82	-0,9232	0,9965	16
Zn	64 67	48,89 27,77	1 1	0,4946	0,87	0,0279	0,9999	10

The calibration graph for Zn in the UF_4 matrix is given in Figure 5.4 as an example of a good calibration curve.

The calibration graph for S in a UF_4 matrix is given in Figure 5.5 as an example of a poor calibration curve.

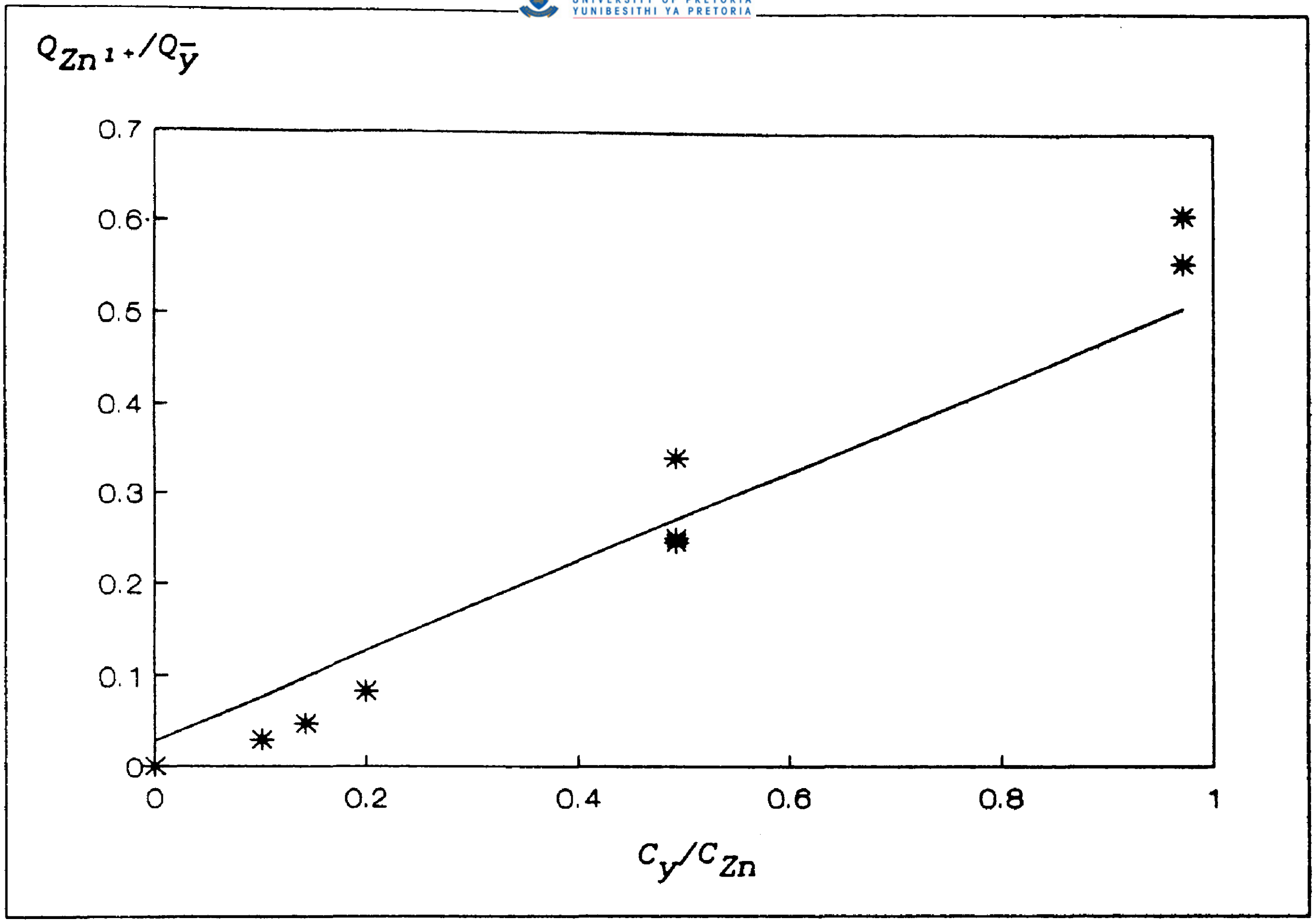


Figure 5.4: Calibration curve for Zn^{1+} *in a* UF_4*/graphite matrix*

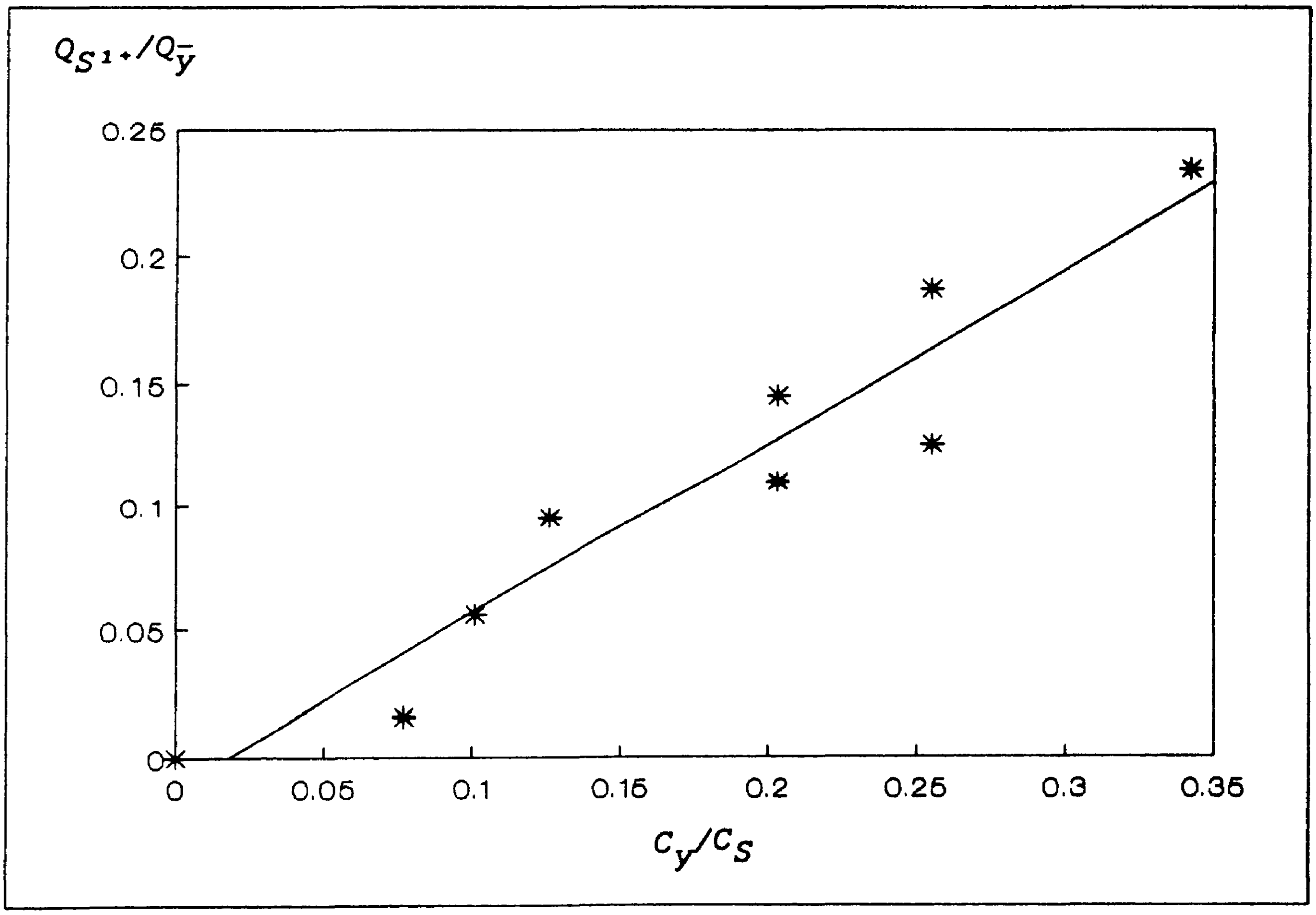


Figure 5.5: Calibration curve for S^{1+} *in* UF_4*/graphite matrix*

The poor fit of data for S is manifested through the relatively large error in the slope (α = 26,9%) and the high value obtained for S in the blank UF_4. Where blank values are reasonably high, uncertainties in these values are reflected in all other data points. This also happens when standards are added to a quantity which is not known in absolute terms.

The value of n in Table 5.5 is an indication of the number of data points used to construct the calibration curves, where each data point is taken as a single analysis. The value for the blank is also incorporated as a data point.

5.3.3 Relative Sensitivity Factors (RSF's) - UF_4

For the impurity elements investigated in a UF_4 matrix, various physico-chemical properties were studied in order to find a qualitative solution for the very high RSF's obtained for P (25,7454) and Cl (20,0095) listed in Table 5.5. Properties such as first and second ionisation potentials (I_p), bond strength (B_s) of the F-X species, heats of formation (H°_f) of gaseous atoms from elements in their standard states, heat of vaporisation (H°_{vap}), electronegativity (E_{neg}), melting points (M_p) and boiling points (B_p) were studied [28]. No specific physico-chemical property can be singled out to explain anomalies in RSF's as each property plays a role within the plasma. When the melting points and heats of vaporisation are compared between the various elements, it is apparent that P and Cl have the lowest values. However, these elements also have of the highest E_{neg} and ionisation potentials.

5.4 Semi-quantitative analysis

5.4.1 50% Transmission intercept method

This method is more time consuming than the appearance level method (see page 132) but is still quicker than setting up the MD100 microdensitometer to obtain analytical data. Instruments required to perform this method are a Hilger & Watts* microphotometer Model L-500-2 equipped with a carriage to hold a photographic plate and a Fluke# multimeter. Many of the principles and preliminary procedures discussed in detail for the appearance level method also apply to this method. However, only the operational procedure will be discussed below.

The marked photographic plate is positioned and the lens focused, once the light of the photocell has been switched on. A clear plate region of at least 5mm in diameter is made on the photographic plate where there are no spectral lines of interest, by scraping away the emulsion on the photographic plate. This spot will serve as the 100% transmission region in order to calibrate the multimeter.

The intensity of the light is adjusted by means of the photocell amperage so that when the beam of light is mechanically shut off

* Hilger & Watts Ltd, 98 St Pancras Way, Camden Road, London NW1.

John Fluke MFG. Co. INC, P.O. Box 43210, Mountlake Terrace, Everett, Washington, 98043, U.S.A.

there is 0% transmission of light and when the beam of light passes through the clear plate region there is a 100% transmission of light through the photoplate. The Fluke digital multimeter is coupled to the photocell output using its 1 volt scale so that 0% transmission is zero volt on the multimeter and 100% transmission is 1,0 volt on the multimeter. The second decimal scale is sufficient for this method as a reading of 0,65 volt on the multimeter gives a reading of 65% transmission of light through the spectral line. Dark spectral lines on the photoplate will have lower percentage transmission of light through them than lighter spectral lines. The 50 % transmission intercept method can now be implemented.

An element of known concentration is used to obtain a k-factor e.g. U or Y. The $^{234}U^{2+}$ spectral line at m/e 117 is used as internal standard or the $^{89}Y^{1+}$ or $^{89}Y^{2+}$ spectral lines at m/e 89 and 44,5, respectively, can be used as internal standard if Y is present in the sample. A transmission curve is obtained by plotting on the y-axis, using ordinary graph paper, the multimeter reading multiplied by 100 to obtain a percentage transmission for each spectral line on the photographic plate. This is plotted against the natural logarithm on the x-axis of the applicable exposure value of each spectral line on the photographic plate i.e. % T on the y-axis and ln Q on the x-axis. From this transmission curve, the exposure value at 50 % transmission is read off the graph paper and is used in the general formula to obtain a k-factor.

The same procedure is followed as above to obtain a transmission curve for an element X of interest. The exposure value at 50 % transmission is used, together with the k-factor obtained from *the internal reference to obtain the concentration value, C_x, of element X. However, this concentration is only for that particular isotope of element X. In order to obtain the total concentration C_x of element in the sample, the isotopic abundance of the applicable isotope measured must be incorporated.*

This method is suitable to obtain concentration values for impurity elements in a sample where no relative sensitivity factors are available. In this case the RSF is taken as unity and the final result obtained differs from the true value by about a factor of two or three. The fact that no background correction has been incorporated must be borne in mind. This method can be utilised with high and low concentrations of impurity elements as long as there is a spectral line that can produce a workable transmission curve. Both the semi-quantitative methods are extremely useful for analysing uranium samples where no standard is available. In this case the uranium is taken as the internal standard and used to quantify impurity elements.

5.4.2 *Appearance level method*

This method is the more reliable method of the two used for semi-quantitative analysis. However, its interpretation differs from analyst to analyst as will be illustrated below. The only instrument required to perform this method is a microscope which is equipped with a carriage to hold a photographic plate. Whilst looking through the eye-piece of the microscope, the analyst must be able to move the carriage holding the photographic plate, along both the x- and y-axes. The x-direction gives the analyst the opportunity to view the spectrum on the photographic plate in its entirety whereas movement in the y-direction focuses on a specific area of the photoplate and the number of different exposures in the form of spectral lines can be counted. This last step is the essence of the method.

If an uranium oxide sample, for example U_3O_8, has been mixed with graphite powder spiked with the internal reference standard, Y, of known concentration, then the U and/or Y are used as the elements of known concentration. A prerequisite for using the U line as reference, is that the isotopic composition is known. If the U is natural, then the concentrations of the various isotopes are known and can be used as reference concentrations. This is shown below as an example.

Uranium used: natural
isotopic abundance (converted to mass percent): 238 = 99,286
235 = 0,710
234 = 0,0055
thus concentration of: ^{238}U = 992 860 µg $^{238}U/g\ U_3O_8$
^{235}U = 7 100 µg $^{235}U/g\ U_3O_8$
^{234}U = 55 µg $^{234}U/g\ U_3O_8$

The concentration of the ^{234}U isotope of uranium is normally used as it has a value similar to impurity levels in the U_3O_8.

The above concentrations can be expressed in general ppm terms as µg of the U isotope per total mass of U (in grams). For natural uranium in U_3O_8 the concentrations are:

^{238}U = 882 425 ppm
^{235}U = 6 167 ppm
^{234}U = 47,8 ppm

When graphite powder spiked with a known concentration of Y is mixed with the U_3O_8, it is done in the ratio of five parts U_3O_8 to one part graphite by mass. This was shown on page 30. The concentration of the Y in the graphite is typically 80 µg Y/gC. When mixed with U_3O_8, the concentration of Y relative to uranium is approximately 20 µg Y/gU. These two concentrations are used when applying the appearance level method.

When a set of spectral lines belonging to a specific element on the photographic plate is investigated under the microscope, dark lines at longer exposures up to light lines at shorter exposures, are observed. At very short exposures, no spectral lines are detected depending on the concentration level of that element in the sample.

The faintest detectable spectral line is called the appearance line. According to the exposure pattern used, this appearance line thus has a specific appearance exposure. The appearance exposure can thus be defined as that exposure necessary for a specific impurity element present at a certain concentration level to become visible to the analyst. This is where the difference in interpretation of the appearance level method varies from analyst to analyst. What might be the appearance exposure for one analyst is not necessarily that for the other analyst.

When performing semi-quantitative analyses with this method, both the Y^{1+} and Y^{2+} lines at masses 89 and 44,5, respectively, are scrutinized to obtain appearance exposures. Similar to quantitative analysis procedures, the mean of these two values is obtained:

$$Q_{\bar{y}} = \frac{Q_{y^{1+}} + Q_{y^{2+}}}{2}$$

When applying the general formula for spark-source mass spectrometry,

$$\text{concentration (C)} = \frac{\text{k-factor}}{\text{exposure (Q)}}, \qquad \ldots\ldots\ldots\ldots\ldots\ (1)$$

the k-factor for Y , K_y, can be obtained:

$$K_y = C_y . Q_{\bar{y}} \qquad \ldots\ldots\ldots\ldots\ldots\ (2)$$

where:

C_y is the concentration of the internal standard Y, relative to the U content, i.e. typically 20 µg Y/gU in the above example, and

$Q_{\bar{y}}$ is the mean appearance exposure of the internal standard.

For an unknown impurity element X present in the U_3O_8 sample, the appearance exposure, Q_x, is determined using the same method as described above.

Using the above Q_x and K_y from equation (2) in equation (1), the concentration C_x of element X relative to the internal standard is determined:

$$C_x = \frac{K_y}{Q_x} \qquad \dots\dots\dots\dots\dots \quad (3)$$

If the internal standard is not present, the U spectral lines are used in exactly the same way. However, only the $^{234}U^{2+}$ spectral line at m/e 117 is suitable for use. The concentration of an element X is then expressed relative to the ^{234}U isotope.

This method is a quick way to obtain a concentration for an element without using relative sensitivity factors. The result can differ by a factor of two or three compared to the use of relative sensitivity factors (RSF's). In the above case, the sensitivity of an element X relative to an internal standard is taken as unity. If a RSF does exist for an element X relative to Y in a specific matrix, then it can be used together with the usual formula given below which was derived on page 98:

$$C_x = \frac{RSF \, . \, C_y}{\frac{Q_x}{Q_{\bar{y}}}} \qquad \ldots\ldots\ldots\ldots\ldots \quad (4)$$

The appearance exposure of element X, Q_x, is expressed as a ratio together with the mean appearance exposure of the internal standard, $Q_{\bar{y}}$. The concentration C_x obtained for element X is only the concentration of that particular isotope of element X. In order to obtain the total concentration of the element, the concentration obtained for that particular isotope measured, is divided by its isotopic abundance and multiplied by 100 to cancel the percentage.

CHAPTER SIX

EVALUATION OF THE METHOD

6.1 Statistical significance of results

6.1.1 Statistical approach

Data interpretation is based on the graphic method [29, 30]. This incorporates the use of calibration lines which are obtained from plotting the instrument signal, y, against the concentration, x, of an element. The relationship between x and y can be derived by linear regression using the standard formula:

$$y = mx + c \qquad \text{..............} \quad (1)$$

where:

m is the slope of the calibration line, and
c is the intercept of the y-axis.

The general spark-source mass spectrometry formula [8] can be interpreted on this basis:

$$C_x = \frac{K_x}{Q_x} \qquad \text{..............} \quad (2)$$

where:

C_x is the concentration of element X,
K_x is a constant and
Q_x is the exposure value at 50% transmission of element X.

Equation (2) can be rewritten in the form of equation (1) as follows:

$$\frac{1}{Q_x} = K_x \cdot C_x$$

The intercept c, on the y-axis of equation (1) is taken as zero and is explained later on in this section (see page 139).

The same general formula applies for the internal standard Y, namely:

$$C_y = \frac{K_y}{\bar{Q}_y} \quad \ldots\ldots\ldots\ldots\ldots \quad (3)$$

$\bar{Q}_y$ is the mean exposure value of Y for the charge states 1+ and 2+ (see page 29).

Combining equations (2) and (3) gives:

$$\frac{Q_x}{\bar{Q}_y} = \frac{K_x}{K_y} \cdot \frac{C_y}{C_x} \quad \ldots\ldots\ldots\ldots \quad (4)$$

where:

$\frac{Q_x}{\bar{Q}_y}$ is the instrument signal, expressed as the ratio between the exposure value, Q_x, of element X at 50% transmission and the exposure value $\bar{Q}_y$, of the internal reference standard, Y, at 50% transmission;

$\frac{C_y}{C_x}$ is the ratio between the concentration of the internal reference standard, Y, and the concentration of element X which is given in µg X/gU; and

$\frac{K_x}{K_y}$ is the slope, expressed as the relative sensitivity factor (RSF) [18, 31] of an element X, relative to the internal reference standard, Y.

The concentration of the internal standard, Y, is taken as 20 µg Y/gU when analysing unknown U_3O_8 samples and 132 µg Y/gU when analysing unknown UF_4 samples. The choice of these concentrations of the internal standard is comprehensively described on pages 29, 103 and 122.

The concentration of an element X varies according to the range of graphite standards prepared. The choice of these ranges is comprehensively described on page 103 for a U_3O_8*/graphite matrix and on page 122 for a* UF_4*/graphite matrix.*

The instrument signal, $Q_x/Q_{\bar{y}}$*, is obtained when doing data interpretation and is taken as the intercept at a 50% transmission of the Hull function plot. This is described on page 36.*

The origin (0;0), of the calibration graph is also incorporated in the calibration line. This is shown as follows:
When C_x *tends to infinity, then the expression* C_y/C_x *tends to zero when* C_y *is taken as constant. From equation (2), when* C_x *tends to infinity, then* Q_x *tends to zero. Likewise, the expression* $Q_x/Q_{\bar{y}}$ *tends to zero when* $Q_{\bar{y}}$ *is taken as constant because* C_y *is constant. Thus both expressions tend to the origin (0;0) when* C_x *tends to infinity. This verifies the use of the origin as a data point when compiling calibration graphs.*

Linear regression formulae [29] (see Appendix A on page 174) are used to determine the standard error, s_m*, in the slope of the regression line. The confidence limits of the slope, expressed as* α*, is given by the following formula [32]:*

$$\alpha = s_m \cdot t \qquad \text{..............} \quad (5)$$

where:
s_m *is the standard error of the slope, and*
t is the Student's t-value [33] at a 95% confidence level (CL) with (n-2) degrees of freedom where n is the number of data points (x;y) used to draw up the calibration graph.

The parameters RSF, α*,c, r and n obtained from the regression line are given in Table 5.2 (see page 111).*

6.1.2 Propagation-of-errors approach [30, 34]

This method is used when determining the concentration C_x, of an element X, in an unknown U_3O_8 sample. Equation (4) can be rewritten as follows:

$$C_x = \frac{(RSF \pm \alpha).(C_y \pm c_y)}{\dfrac{Q_x}{\overline{Q}_y} \pm 2s} \quad (95\%\ CL) \quad \ldots\ldots\ldots\ldots \quad (6)$$

The confidence limits α, of the slope or relative sensitivity factor is obtained from Table 5.2 on page 111. Likewise, the applicable relative sensitivity factor RSF, is given in Table 5.3 (see page 120). The concentration of the internal standard, Y, given by C_y, is taken as 20 μg Y/gU where graphite powder has been spiked with 80 μg Y/gC. This graphite powder, called UFY80, is used as electrode material when analysing unknown U_3O_8 samples. The error in C_y, given by c_y, is taken as 0,5% which is the maximum imprecision of a 1 000 μl varipette used to dispense the Y ICP standard solution. The precision of the Mettler H10T mass balance used to weigh out the required mass of graphite powder is 0,1 mg which gives an error of 0,002% when 5 grams of graphite is used. The Y ICP standard solution is certified to <0,01% and the error is not significant. These errors can be ignored statistically and only the error in the varipette, 0,5%, is taken as c_y [38].

The precision of the method is also known and is given in Table 6.1 (see page 147). For a single analysis of an unknown U_3O_8 sample, the error coupled to the instrument signal, $Q_x/\overline{Q}_y$, for element X is taken as twice the standard deviation, 2s [35, 38]. This is based on the assumption of a normal distribution of results where an analysis result has a 95% chance of lying within two standard deviations of the mean.

When considering the general error formulae used in composite errors, the following applies [36, 37]:
For a number of quantities, n, with means $\bar{x}_1$, $\bar{x}_2$, ----, $\bar{x}_n$, with standard errors α_1, α_2, ---, α_n, the standard error of

any function of $\bar{x}_1$, $\bar{x}_2$, ---, $\bar{x}_n$, namely, $f(\bar{x}_1, \bar{x}_2, ---, \bar{x}_n)$ is

given by α, where $\alpha^2 = \left(\frac{\partial f}{\partial \bar{x}_1}\right)^2 \alpha_1^2 + \left(\frac{\partial f}{\partial \bar{x}_2}\right)^2 \alpha_2^2 + --- + \left(\frac{\partial f}{\partial \bar{x}_n}\right)^2 \alpha_n^2$

The quotient of two mean values is given by:

$$f(\bar{x}_1, \bar{x}_2) = \frac{\bar{x}_1}{\bar{x}_2}$$

thus $\dfrac{\partial f}{\partial \bar{x}_1} = \dfrac{1}{\bar{x}_2}$ and $\dfrac{\partial f}{\partial \bar{x}_2} = -\dfrac{\bar{x}_1}{\bar{x}_2}$

This gives $\alpha^2 = \left(\frac{1}{\bar{x}_2}\right)^2 \alpha_1^2 + \left(-\frac{\bar{x}_1}{\bar{x}_2}\right)^2 \alpha_2^2$

$$= \frac{1}{\bar{x}_2^4} (\bar{x}_2^2\alpha_1^2 + \bar{x}_1^2\alpha_2^2)$$

Therefore $\alpha = \dfrac{1}{\bar{x}_2^2} \sqrt{\bar{x}_2^2\alpha_1^2 + \bar{x}_1^2\alpha_2^2}$ .... (7)

The product of two mean values is given by:

$$f(\bar{x}_1, \bar{x}_2) = \bar{x}_1 . \bar{x}_2$$

$$\text{thus } \frac{\partial f}{\partial \bar{x}_1} = \bar{x}_2 \quad \text{and} \quad \frac{\partial f}{\partial \bar{x}_2} = \bar{x}_1$$

This gives $\alpha^2 = \bar{x}_2^2\ \alpha_1^2 + \bar{x}_1^2\ \alpha_2^2$

$$\text{and} \qquad \alpha = \sqrt{\bar{x}_2^2\ \alpha_1^2 + \bar{x}_1^2\ \alpha_2^2} \qquad \ldots\ldots\ldots\ldots\ldots \quad (8)$$

Applying the above equations (7) and (8) to equation (6), the standard error, s_{C_x}, of the concentration of element X in the unknown sample is derived.

$$\text{Thus } s_{C_x} = \frac{1}{\left(\frac{Q_x}{Q_y}\right)^2} . \sqrt{\left(\frac{Q_x}{Q_y}\right)^2 . (C_y^2 \alpha^2 + RSF^2 c_y^2) + (RSF.C_y)^2 . (2s)^2} \quad \ldots\ldots \quad (9)$$

The final result of element X is reported as:

$C_x \pm s_{C_x}$ (95 % CL)

This gives the confidence interval derived using the propagation-of-errors method at a 95 % confidence level.

6.1.3 Precision

In order to determine the precision coupled to the analysis of U_3O_8/graphite matrix samples using spark-source mass spectrometry, three of the prepared graphite standards with concentrations of 1,0; 10,0 and 50,0 µg X /gU were each analysed six times (i.e. n = 6) mixed with the base U_3O_8 (see page 103). The results obtained are tabulated in Table 6.1 on page 147. The precision that is obtained is for both the instrument and the analyst.

The standard error at a 95% confidence level (CL) was determined using the following formula [37]:

$$\bar{x} \pm \frac{t.s}{\sqrt{n}} \text{ at } 95\% \text{ CL} \qquad \ldots\ldots\ldots\ldots\ldots \ (1)$$

where:

$\bar{x}$ is the mean of the six analyses of one standard;
s is the standard deviation of the six analyses; and
t is the Student's t-value taken at a 95% confidence level using (n − 1) degrees of freedom (ν).

Before the above formula could be used, the data obtained had to be subjected to the Dixon outlier test [38, 39, 40, 41] in order to ascertain whether there were any "mavericks". The Dixon outlier test assumes that the parent population from which the measurements are obtained is normally distributed.

One way of assessing a suspect measurement is to compare the difference between it and the measurement nearest to it in size with the difference between the highest and lowest measurements. The ratio of the differences is known as Dixon's Q and is given as Q_{calc} in the following basic formula:

$$Q_{calc} = \frac{|\ \text{suspect value} - \text{nearest value}\ |}{(\text{largest value} - \text{smallest value})} \qquad \ldots\ldots \ (2)$$

The critical values of Q, given as Q_{tab}, are taken from the table of critical values for Q at a 95% confidence level (CL).

The following reasoning is applied in the Dixon test:
If $Q_{tab} \geqslant Q_{calc}$, then the suspect value is retained;
if $Q_{calc} > Q_{tab}$, then the suspect value is rejected.
From the table of critical values of Q, the sample size in this case is taken as six.

It is important to note that at a 95% CL there is still a 5% chance of incorrectly rejecting the suspect value. When measurements are repeated only a few times rejection of one value makes a great difference to the mean and standard error. This has a considerable effect on the estimation of the precision. The importance of caution in rejecting outliers cannot be over-emphasised. There is also the possibility of two suspect values which leads to masking in the application of the Dixon Q-test.

Using the above approach, suspect values were rejected for a number of elements from each of the standards. This is shown in Table 6.1 where n = 5. For Mo^{1+} (n = 4) and Sm^{1+} (n = 3), the experimental data obtained was limited as the spectral lines on the photographic plate could not be measured in all the cases.

An assessment of the results tabulated in Table 6.1 reveals that most of the standard errors at a 95% CL are below 20% with the exception of a few cases which will be explained below. This is in accordance with values reported by many other authors [31] who have used electrical detection, radio frequency (RF), glow discharge (GD) and other types of spark-source mass spectrometers for analysing U samples.

The first few elements in Table 6.1, namely B, Mg and Al, have high standard errors at all the concentration levels. This is ascribed to interference of their spectral lines at masses 10 and 11 for B, 12,5 for Mg and 13,5 for Al, due to the spectral lines of the matrix component C at masses 12 and 13. The C spectral lines, being from the major constituent of the sample, are intense and dispersed in the region surrounding them, thus affecting the adjacent spectral lines and their precision, irrespective of concentration.

The standard errors for most of the elements at a concentration level of 1 µg X /gU are relatively high. This is a result of unreliable data obtained from the transmission curves. Only a few points could be utilised in the Hull function plot as most of these were light points. This could also be ascribed to the fact that at this concentration level, the detection limit for some of the elements is reached. Typical examples affected in this manner are Mn^{1+}, Zn^{1+}, Zr^{1+} and the heavier elements such as the rare earths Sm, Eu and Dy.

The high standard errors at a 95% CL for the heavier elements, such as the rare earths at a concentration level of 1 µg X /gU, is ascribed to the fact that these elements provide small ion yields of the various charge states resulting in poor transmission curves. The atomic size of these elements affects the number of ions entering the ion source due to collisions. These ions also have a smaller velocity down the flight tube of the mass spectrometer. All these factors have a decisive impact on the nett total of ions yielded at the photographic plate.

The very high standard error for Mo^{1+} at a 95% CL, namely 84,1%, can be ascribed to the previous reasons (poor ion yield, near the low concentration detection limit, as well as the small number of useful data points). When applying the formula to determine the standard error at a 95% CL, the degrees of freedom (ν) is given as ($n - 1$), i.e. 3 where $n = 4$, which is relatively small. This means that the standard deviation, s, is multiplied by a factor 1,59 (3,182/2) giving a higher standard error. As n gets larger, the factor of $t/\sqrt{n}$ gets smaller, thus reducing the standard error in a significant way.

The standard errors for Ca^{2+} and Si^{1+} are relatively high as the Ca^{2+} spectral line was measured as a doublet and the Si^{1+} spectral line was measured as a triplet. The analyst has to set windows around these lines and this affects the background surrounding the spectral lines which are under scrutiny. This leads to a weaker precision at all concentration levels.

The high standard error for Ni^{1+} at 95% CL at a concentration of 50 µg Ni /gU, namely 34,2%, is verified as follows. From the raw data obtained, there is one data point out of the set of six ($n = 6$) that appears to differ from the remainder. However, when applying the Dixon outlier test to this data point, the test shows that this data point cannot be taken as an outlier and must thus be retained. This leads to the high standard error. If the Dixon outlier test had shown that this point could be rejected, the precision would have been 15,9% for the remainder of the data points ($n = 5$). This could be interpreted as a possible limitation of the Dixon outlier test.

The precision values obtained are used together with the relative sensitivity factors (RSF's) when analysing the unknown U_3O_8 samples where the error in the instrument signal is taken as twice the standard deviation.

TABLE 6.1: Precision for U_3O_8

Element	Charge State	C_x = 1µg X /gU		C_x = 10µg X /gU		C_x = 50µg X /gU	
		Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n
B	1	27,6	6	24,8	6	36,1	6
Mg	2			10,3	5	40,4	6
Al	2			24,7	6	22,6	6
Si	2	38,6	6	11,1	6	16,6	6
Si	1			25,3	6	35,5	6
Ca	2	12,0	6	24,8	6	29,5	6
Ti	2			6,1	5	13,2	6
Ti	1	21,2	6				
V	2			13,9	6	15,9	6
V	1	7,6	6	10,5	6	8,8	6
Cr	2			10,8	6	10,7	6
Cr	1	17,7	6	14,0	6	18,6	6
Mn	2			16,3	6	22,0	6
Mn	1	29,7	6	19,1	6	19,1	6
Fe	2			19,0	6	12,8	6
Fe	1	18,9	6	15,5	6	15,4	6
Co	2			11,2	6	17,2	6
Co	1	6,6	6	5,0	6	17,7	6
Ni	1	19,3	6	2,6	6	34,2	6
Cu	2			7,1	6	17,0	6
Cu	1	15,3	6	15,3	6	19,3	6
Zn	1	32,5	6	8,8	6	21,6	6
Sr	2			10,2	6	17,2	6
Sr	1	18,1	6	9,4	6	15,7	6
Zr	2			8,4	6	15,8	6
Zr	1	36,1	6	6,2	6	11,2	6
Nb	2			10,6	6	15,6	6
Nb	1	18,2	6	10,9	6	5,8	5

Table 6.1: Continued

Element	Charge State	C_x = 1μg X /gU		C_x = 10μg X /gU		C_x = 50μg X /gU	
		Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n
Mo	2			8,6	6	16,2	6
Mo	1	84,1	4	7,1	6	11,2	6
Ru	2			13,9	6	12,2	6
Ru	1			7,7	5	5,0	5
Cd	1			10,4	6	15,3	6
In	1	23,9	6	11,7	6	21,9	6
Sb	2			7,6	6	8,6	6
Sb	1	34,1	6	12,2	6	16,3	6
Ba	2			8,6	6	8,9	6
Ba	1	27,5	6	15,9	6	17,1	6
Sm	2	48,3	5	9,4	6	10,7	6
Sm	1			18,8	3	17,0	6
Eu	2	33,3	6	7,3	6	14,2	6
Eu	1			5,8	6	8,8	5
Gd	2			6,8	5	9,3	6
Gd	1			8,4	5	5,0	5
Dy	2	32,0	5	14,9	6	9,8	6
Dy	1			7,3	5	12,4	6
Bi	2			25,2	6	15,0	6
Th	2	25,8	6	12,9	6	20,2	6

6.1.4 Confidence Intervals - U_3O_8

Confidence limits of the slope, expressed as α, have a significant influence on the relative sensitivity factor (RSF) derived as the slope of the calibration curve. Large α values mean large uncertainties in the RSF's. These uncertainties must be included in the overall errors calculated for the final analysis results. Values of α greater than 20% in Table 5.2 (see page 111) can be ascribed to a number of reasons, of which the important ones are given below.

The value of n has a significant influence on the value of α. This can be demonstrated using equation (5) on page 139 where the t-value is obtained using (n - 2) degrees of freedom at a 95% confidence level (CL). For n = 7, the t-value from the Students t-Distribution Table is 2,571. The standard error in the slope, s_m, must be multiplied by this number in order to obtain the α value and leads to large confidence limits of the slope.

When determining the calibration curve parameters, each analysis of a graphite standard sample was treated as an individual analysis. Thus, when a graphite standard was analysed in triplicate, the value of n was taken as three. This was typically done using the check graphite standards where some elements were analysed for the first time, e.g. Na, P, K and W. Using two such check graphite standards together with the origin (0;0) gives a t-value of 2,571, where n = 7. This means that a standard error in the slope of 20% becomes a confidence limit of 51,4%. A number of elements in Table 5.2 fall into this category, namely Na^{1+} (11%), P^{1+} (8,1%), P^{2+} (13,6%), K^{2+} (7,8%) and W^{2+} (14,5%), where the standard error is given in brackets after each element.

The ion yields of certain elements with specific charge states at their lowest concentration levels are not very good, with the result that poor transmission curves are obtained. Only a few long exposure values are used in the Hull function plot and the rest of the data points are discarded as light points. The charge state differs from element to element depending on the atomisation and ionisation of the particular element. This can be illustrated when plotting characteristic curves of number of ions yielded against charge state. A number of cases in Table 5.2 where α is near or greater that 20 % can be placed into this category, namely K^{2+}, Ru^{2+}, Ba^{1+}, W^{1+}, Sm^{1+}, Mo^{1+} and Sb^{1+}.

Elements with large atomic radii are more prone to collisions and also have a slower velocity down the flight tube. This leads to fewer ions reaching the photoplate. From Table 5.2, elements falling into this category are Sm^{1+}, W^{2+}, Ba^{1+}, Mo^{1+}, Sb^{1+} and Ru^{2+}.

The correlation coefficient, r, in Table 5.2 can also be coupled to a larger α value. Ideally r should be unity, thus values of $r < 0,90$ show that the fit of calibration data to the regression line is seriously affected by a few bad data points. The inclusion of these bad data points is confirmed by applying the Dixon outlier test which shows that these values have to be retained. However, great caution should be exercised in drawing conclusions from the result of repeated applications of the Dixon's test. If a few statistical outliers are found at a certain particular concentration level this is not very serious, but if several outliers occur at different concentration levels, this may be considered as indicating that the regression line and thus the RSF is inaccurate. This would lead to a large spread of data points resulting in a large standard error in the slope, s_m.

Correspondingly, a larger α value is obtained. Elements in Table 5.2 having poor correlations where r <0,90 are Fe^{1+} (r = 0,853) and Ba^{1+} (r = 0,897). This is in spite of n being large for Fe^{1+} (n = 30) and Ba^{1+} (n = 22). Elements in Table 5.2 having correlation coefficients of r <0,95 are the following: Mg^{2+}, Si^{2+}, Ca^{2+}, Mo^{1+}, Sb^{1+} and Sm^{1+}.

For Mg^{2+}, Si^{2+}, Fe^{1+} and Na^{1+} it is significant to note that these elements all have high background concentrations in the blank base U_3O_8 sample. The influence of this high blank concentration on the calibration line is discussed on page 105. This effectively reduces the range on the x-axis of the calibration plot. Typically, for Fe^{1+} the range on the x-axis is from zero to 0,2844. The spread of data points in this case is larger than over a greater range on the x-axis and results in a poor fit of the data points on the regression line. Another reason for Mg^{2+} having an α of 19,3% is the fact that it is measured at m/e 12,5 which lies inbetween the two spectral lines of the major component of the U_3O_8/graphite mixture, namely ^{12}C and ^{13}C at m/e 12 and 13, respectively. Intense fogging on the surrounding background makes the measurements of Mg^{2+} difficult and inaccurate.

When using α values to determine the error coupled to an element's concentration in an unknown U_3O_8 sample, the analyst must exercise great care. In the case of Ba^{1+} (23,0%) and Sm^{1+} (45,0%), the analyst should avoid using these charge states, and should rather use the other charge states where the α values are more acceptable. The same argument applies for W^{2+} (40,3%).

The α value for the impurity elements in a U_3O_8/graphite matrix are tabulated in Table 5.2. However, these have also been given as a visual presentation in the form of two periodic tables, the first for the singly charged species, Figure 6.1, and the other for the doubly charged species, Figure 6.2. It is demonstrated that the appropriate application of the guidelines for quantification enables the acquisition of analytical data within very acceptable confidence intervals for most of the selected elements.

6.1.5 Confidence Intervals - UF_4

The confidence limits of the slope, expressed as α and as a percentage in Table 5.5 on page 127, is a direct measure of the uncertainty coupled to the RSF. The α value for S is the only one which is relatively high (26,9%) for impurities in a UF_4 matrix. This could be attributed to a number of factors of which the most important is the fact that sulphur is measured at mass 32 as a doublet with the main interference being $^{64}Zn^{2+}$. This could influence the data and result in a bigger spread of data points for the calibration curve. This bigger spread implies a larger standard error in the slope, resulting in a large α value. This fact is also supported by the relatively poor correlation coefficient obtained ($r = 0,9575$) for the regression line.

The α value for S could also be influenced by the relatively high background concentration in the blank UF_4 ($C_x = 385,4$ µgS/gU). This value is used together with the concentration of the standard to define the x-value in a data point (x;y) when applying linear regression. The higher the blank concentration, the more influence it has on the C_y/C_x value on the x-axis. The standard error for S in the blank UF_4 at a 95% confidence level (38,74%) is also an indication of the difficulty experienced to obtain reliable data for sulphur in a UF_4 matrix.

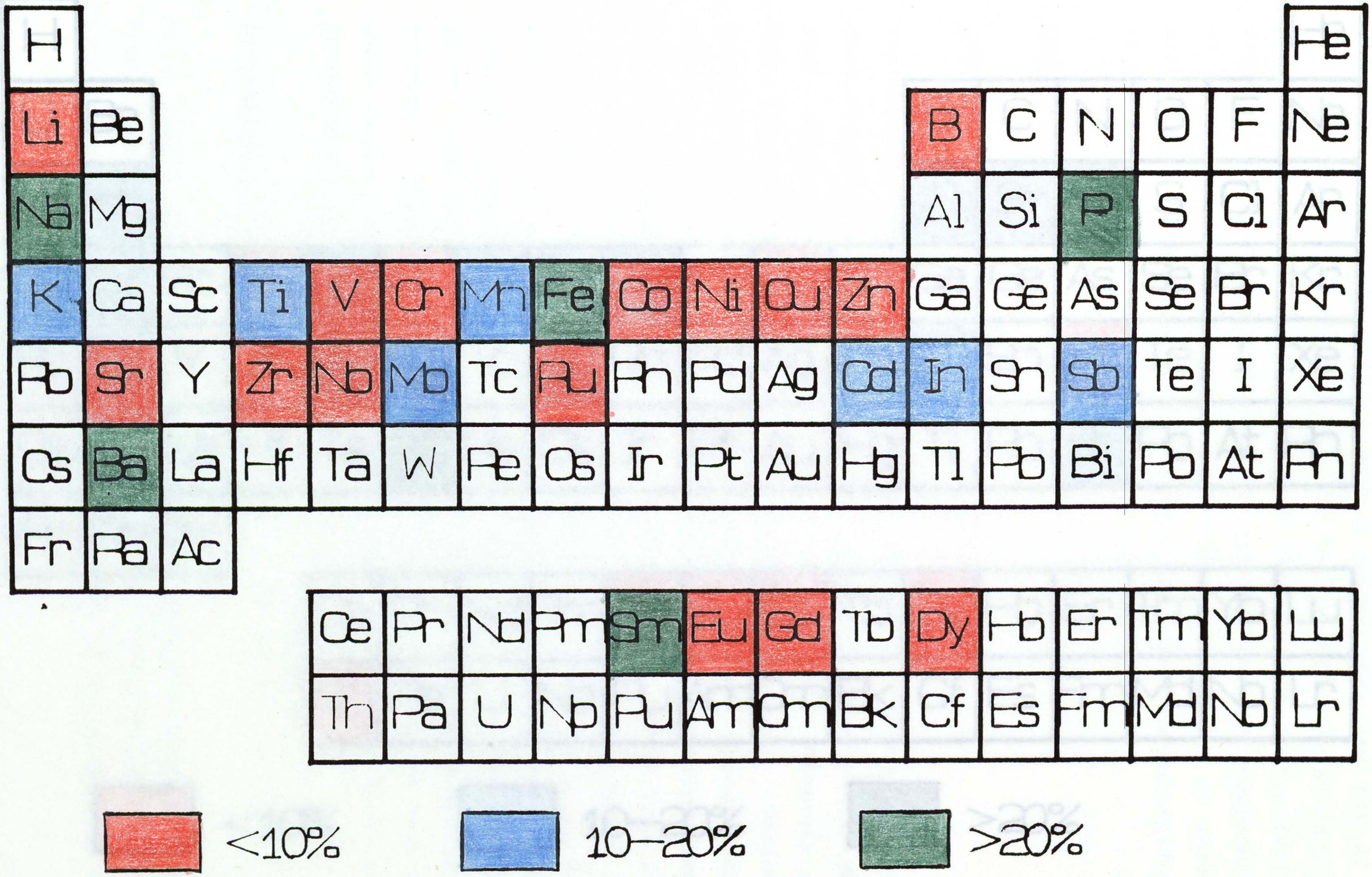
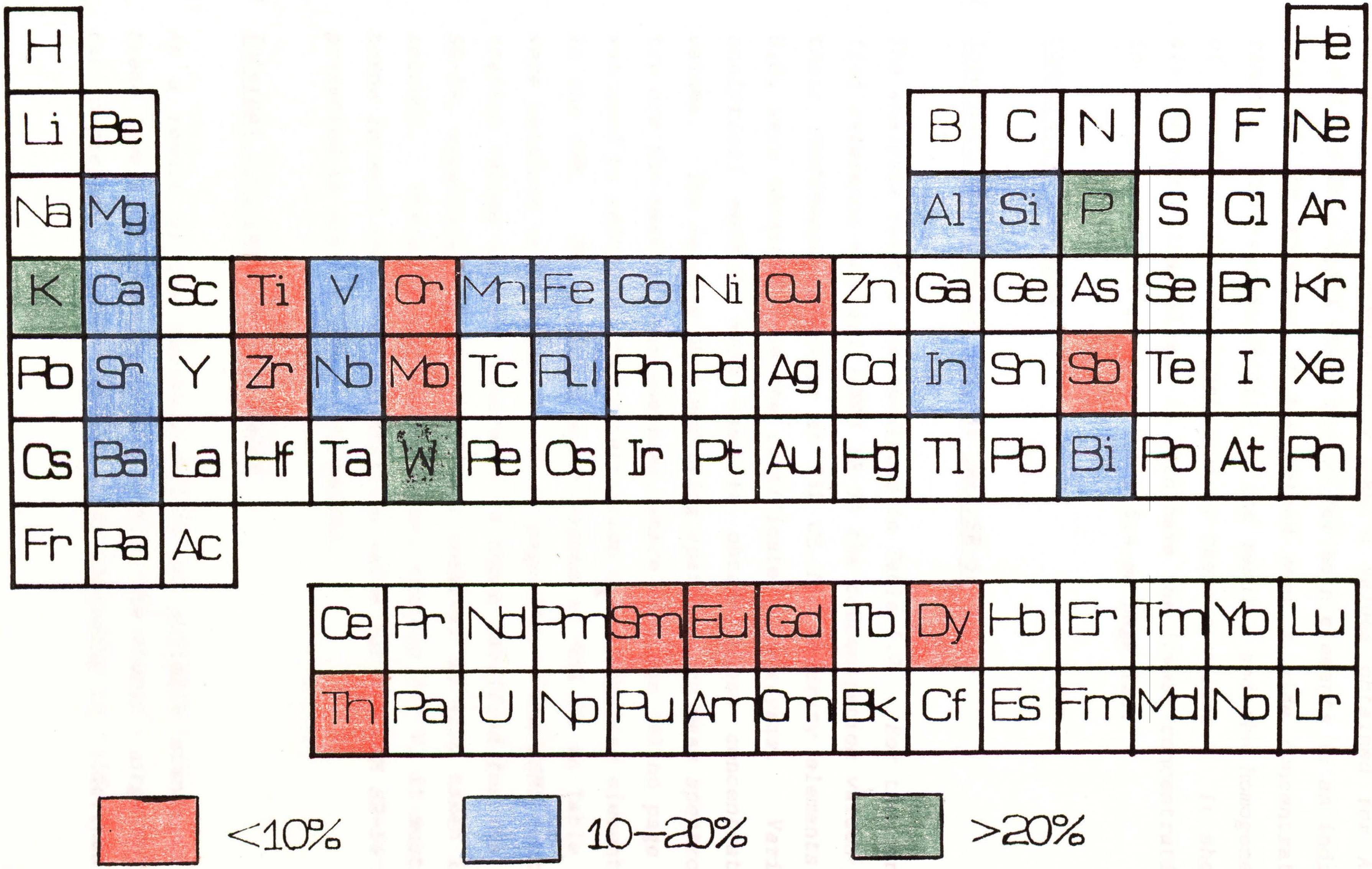


Figure 6.1: Confidence intervals (α) at 95% CL for X^{1+} in U_3O_8



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg 🟦											Al 🟦	Si 🟦	P 🟩	S	Cl	Ar
K 🟩	Ca 🟦	Sc	Ti 🟥	V 🟦	Cr 🟥	Mn 🟦	Fe 🟦	Co 🟦	Ni	Cu 🟥	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr 🟦	Y	Zr 🟥	Nb 🟦	Mo 🟥	Tc	Ru 🟦	Rh	Pd	Ag	Cd	In 🟦	Sn	Sb 🟥	Te	I	Xe
Cs	Ba 🟦	La	Hf	Ta	W 🟩	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi 🟦	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	Sm 🟥	Eu 🟥	Gd 🟥	Tb	Dy 🟥	Ho	Er	Tm	Yb	Lu
				Th 🟥	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

🟥 <10%

🟦 10–20%

🟩 >20%

Figure 6.2: Confidence intervals (a) at 95% CL for X^{3+} in U_3O_8

The other α values in Table 5.5 are all acceptable in the sense that they fall within the precision of the instrument and the analyst. The exceptionally good α values obtained for Al = 0,84% and Zn = 0,87% where n = 10 for both elements is an indication of the accuracy of the method over a wide concentration range. The reproducibility of the results and the homogeneity of the standards are illustrated by these α values. It should also be noted that Al and Zn both have the lowest concentrations in the blank UF_4 as shown in Table 5.4 on page 123.

6.2 Comparative analyses

6.2.1 International standard U_3O_8 No IAEA/SR-54

The analysis results are tabulated in Table 6.2. For the certified reference material (CRM) SR-54 the concentration values and their confidence intervals at 95% CL for impurity elements in U_3O_8 were obtained from the certificate of analysis. Various analytical methods were used to obtain these concentration values. The results obtained using spark-source mass spectrometry are the mean of four analyses, where equation (4) on page 136 was used to calculate the concentration C_X of impurity element X in the CRM. The standard error values at 95% CL in Table 6.2 were obtained using equation (9) on page 142. The SSMS concentration values compare favourably to those certified for the CRM SR-54, especially if the confidence interval is also taken into account. Where differences do occur, notibly for V, it must be borne in mind that the concentration value for the CRM SR-54 was presented as non-certified information.

6.2.2 Internal U_3O_8 certified standards

As a result of the non-availability of suitable standards at trace levels of elements in a U matrix, the Atomic Energy Corporation prepared a series of standards according to guidelines as

TABLE 6.2: Comparison of U_3O_8 CRM SR-54 with SSMS

Element	Certified conc. value (µg X /gU)	Confidence interval at 95% CL	SSMS conc. value (µg X /gU)	Std error at 95% CL
Al	71,3	54,8 - 82,0	70,4	15,9
Co	4,2	4,0 - 4,3	5,2	1,3
Cr	3,6	3,1 - 4,3	2,9	0,8
Cu	5,0	4,2 - 6,7	5,7	0,5
Fe	64,7	46,0 - 77,5	66,2	10,2
K	1,7*	-	3,3	0,7
Mg	0,99*	0,81 - 1,1	1,9	0,8
Mn	15,6	14,3 - 16,9	18,4	3,7
Mo	13,0	9,5 - 17,5	12,7	1,1
Na	2,8*	-	3,9	0,8
Ni	11,4	8,4 - 13,9	10,8	2,0
Si	34,3*	18,0 - 53,5	29,8	7,5
Ti	0,98*	-	1,74	0,37
V	3,7*	-	0,12	0,01
Zn	2,4*	0,89 - 3,2	2,2	0,2

* These values are not certified, but are presented as non-certified information values.

laid down by the New Brunswick Laboratory#. These standards covered a wide concentration range and were prepared in a U_3O_8

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U.S.A.

matrix. The standard with the highest concentration level of impurity elements is called ES 1 and the comparison between the certified value and the concentration value obtained with the spark-source mass spectrometer is given in Table 6.3. The standard with the lowest concentration of impurity elements is called ES 5 and the comparison of results obtained is given in Table 6.7. Standards with concentrations falling inbetween ES 1 and ES 5, named ES 2, ES 3 and ES 4, are given in Tables 6.4, 6.5 and 6.6 respectively.

Of every standard in the ES series of standards, three samplings were each analysed in triplicate. This resulted in each ES series of standards being analysed nine times by a specific analytical technique. The spark-source mass spectrometer (SSMS) concentration values given in Table 6.3 to Table 6.7, are the mean concentrations over nine analyses. These concentration values within an ES standard were also subjected to the Dixon outlier test to ascertain whether there were any outliers before each final mean value was reported.

The formula used to calculate the concentration, C_X, of an impurity element X in each of the ES series of standards is given by equation (4) on page 136. However, this concentration value also contains the contribution from that impurity element also found in the graphite which was used to mix with the U_3O_8 ES series of standards. This has been described on page 108. The concentration levels of impurity elements in the graphite were quantified and deducted from the mean concentration values reported for each of the ES series of standards.

Various analytical methods were used by different laboratories in order to certify these internal U_3O_8 standards, amongst others:

- Inductively coupled plasma (ICP) optical emission spectroscopy (OES),
- Ion chromatography (IC),
- Carrier distillation emission spectroscopy (CDES),
- Atomic absorption spectroscopy (AAS), and
- UV - spectroscopy.

It is beyond the scope of this investigation to go into any detail of how the data obtained for the ES series of standards analysed with the above methods, was evaluated. The certified concentration values and confidence intervals at a 95% CL for the various impurity elements across the ES series of standards given in Tables 6.3 to 6.7 were obtained after the evaluation. These certified values were calculated from the experimental data.

The standard error values at a 95% CL in Tables 6.3 to 6.7 were obtained using equation (9) on page 142. However, the term 2s in this equation was replaced by the term $s.t/\sqrt{n}$ as denoted by equation (1) on page 143. This is in accordance with the fact that the $Q_x/Q_{\bar{y}}$ value used in equation (9) is the mean of several (nine) analyses as previously mentioned in this section. The standard error coupled to this mean $Q_x/Q_{\bar{y}}$ value at a 95% CL is thus derived using equation (1) where n is taken as nine and s is the standard deviation over the nine analyses. The other terms used in equation (9) are identical to those used in equation (6) on page 142 and which were comprehensively described. The use of equation (6) was not warranted as multiple analyses were performed and not just a single analysis.

When comparing the results in Tables 6.3 to 6.7, a number of facts should be kept in mind. The certified values must not be accepted as being the absolute values for particular impurity elements in the series of ES standards. A better representation of the results obtained is given in Appendix C on page 191 where graphs have been compiled for all the impurity elements across the concentration range for each of the analytical methods in comparison to the expected concentration values. In this way anomalies can be detected and comparisons drawn between the spark-source mass spectrometry results and the expected concentration values.

Another interesting fact to consider is whether there is a meaningful difference between a certified value of, for example, 0,1 µg Cd/gU and a SSMS value of 0,64 µg Cd/gU, as reported in Table 6.7. Both these values are less than 1 µg Cd/gU and at these trace levels the detection limits of certain analytical instruments have to be considered. The same could be true for Fe in Table 6.4 where the certified value is given as 208 µg Fe/gU and the SSMS value is given as 264 µg Fe/gU. In view of the various confidence intervals for these two values, it is clear that the analyst should not compare exact values with each other but also take cognicance of the confidence limits coupled to a result when assessing such data.

The SSMS concentration value obtained for Ca across the ES series of standards is higher than the certified concentration values. The higher value could possibly be coupled to an incorrect relative sensitivity factor (RSF) for Ca. This can be seen in the graph for Ca in Appendix C where the graph for SSMS (method B) lies above the dotted line which represents the true concentration values. The very high value for Ca obtained for the ES 1 standard with SSMS was also obtained by three other analytical techniques, namely A, C and D. It has not been possible to confirm the reasons for this difference. Ca is a difficult element to determine with spark-source mass spectrometry and the investigation has not been persued for this element.

The SSMS concentration value obtained for Th across the ES series of standards is higher than the certified concentration values reported for ES 1, ES 2 and ES 3, although no confidence intervals were reported for these values. However, the SSMS results compare favourably to the expected values as shown in the graph in Appendix C.

It should be noted from the graphs in Appendix C that the mass spectrometry results in general, compare remarkably well with the expected standard values.

Table 6.3: Comparison of U_3O_8-Standard ES 1 with SSMS

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error at 95% CL
Al	234	189 - 279	242	43
B	5,7	5,0 - 6,4	4,9	1,0
Bi	14,3	11,6 - 17,0	13,1	3,0
Ca	272	245 - 299	416	110
Cd	5,5	5,0 - 6,1	6,0	1,3
Co	26,6	23,7 - 29,5	28,8	3,5
Cr	125	77 - 174	154	27
Cu	104	84,4 - 124	120	21
Dy	0,56	0,43 - 0,69	0,71	0,24
Eu	0,56	0,44 - 0,68	0,69	0,16
Fe	827	663 - 990	972	191
Gd	0,64	0,41 - 0,87	0,85	0,34
In	6,2	4,4 - 7,9	8,9	1,6
K	536	481 - 591	379	112
Li	11,5	9,31 - 13,7	13,2	3,8
Mg	56,2	48,5 - 63,9	49,8	14,6
Mn	55,3	47,5 - 63,2	65,1	15,5
Mo	54,6	46,1 - 63,1	59,4	7,3
Ni	233	209 - 259	243	47
Sb	11,2	9,2 - 13,1	13,8	2,8
Si	206	169 - 244	221	65
Sm	0,60	0,51 - 0,69	0,62	0,17
Th	3,4	-	11,0	1,7
Ti	52,5	39,9 - 65,1	56,4	12,5
V	5,08	3,97 - 6,19	5,40	0,38
W	13,3	11,4 - 15,2	12,7	5,0
Zn	247	207 - 287	261	41
Zr	59	-	55	6,6

Table 6.4: Comparison of U_3O_8-Standard ES 2 with SSMS

Element	Certified conc value (μg X /gU)	Confidence interval 95 % CL	SSMS conc value (μg X /gU)	Std Error at 95% CL
Al	115	93 - 137	120	24
B	3,8	3,3 - 4,3	3,5	0,7
Bi	5,3	4,2 - 6,3	5,6	1,5
Ca	108	97 - 119	163	32
Cd	2,7	2,4 - 3,0	3,0	0,7
Co	13,5	12,0 - 14,9	13,9	1,1
Cr	59	36 - 82	65	11
Cu	54,1	43,7 - 64,4	58,3	5,7
Dy	0,56	0,43 - 0,69	0,69	0,16
Eu	0,39	0,30 - 0,48	0,49	0,14
Fe	208	165 - 251	264	53
Gd	0,47	0,29 - 0,65	0,64	0,42
In	5,3	3,8 - 6,8	6,4	1,1
K	180	162 - 199	171	35
Li	9,51	7,70 - 11,3	10,8	3,1
Mg	21,8	18,7 - 24,8	22,9	6,2
Mn	25,1	21,6 - 28,7	29,0	4,5
Mo	2,0	1,7 - 2,4	2,4	0,6
Ni	97,4	87,3 - 107	92,0	11,1
Sb	8,0	6,6 - 9,4	10,0	1,9
Si	75	59 - 90	77	17
Sm	0,59	0,50 - 0,68	0,66	0,32
Th	0,6	-	5,5	0,58
Ti	25,2	19,1 - 31,2	26,7	4,4
V	2,03	1,55 - 2,51	2,18	0,25
W	5,7	5,0 - 6,4	5,3	2,37
Zn	98,4	82,2 - 115	95,9	14,1
Zr	49		46	5

Table 6.5: *Comparison of U_3O_8-Standard ES 3 with SSMS*

Element	Certified conc value (μg X /gU)	Confidence interval 95 % CL	SSMS conc value (μg X /gU)	Std Error at 95% CL
Al	68	54 - 81	68	18
B	1,4	1,2 - 1,6	1,3	0,3
Bi	3,8	3,0 - 4,6	4,9	1,7
Ca	72	65 - 79	99	20
Cd	1,0	0,9 - 1,2	1,3	0,3
Co	5,1	4,5 - 5,7	5,8	0,6
Cr	28	17 - 40	29	7
Cu	34,0	27,4 - 40,5	38,3	5,6
Dy	0,48	0,36 - 0,60	0,54	0,21
Eu	0,39	0,30 - 0,48	0,50	0,11
Fe	72	56 - 89	65	16
Gd	0,22	0,12 - 0,32	0,74	0,20
In	4,3	3,0 - 5,5	5,7	1,0
K	87	78 - 96	79	22
Li	7,12	5,75 - 8,49	7,86	2,1
Mg	11,4	9,8 - 13,0	15,9	4,9
Mn	12,1	10,4 - 13,8	13,3	2,1
Mo	1,2	1,0 - 1,4	1,3	0,3
Ni	53,9	48,3 - 59,6	52,2	8,2
Sb	3,9	3,1 - 4,7	5,2	1,2
Si	44	33 - 54	63	21
Sm	0,43	0,36 - 0,50	0,56	0,20
Th	0,3	-	3,0	0,5
Ti	10,9	8,3 - 13,6	10,1	2,0
V	1,01	0,74 - 1,28	1,22	0,12
W	4,2	3,6 - 4,7	3,7	1,6
Zn	54,8	45,6 - 63,9	62,7	7,6
Zr	49	-	46	6

Table 6.6: Comparison of U_3O_8-Standard ES 4 with SSMS

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error at 95% CL
Al	23	19 - 28	27	5
B	0,6	0,5 - 0,7	0,8	0,1
Bi	2,5	1,9 - 3,0	3,1	0,8
Ca	23,8	21,2 - 26,4	34,1	5,7
Cd	0,5	-	1,5	0,4
Co	2,7	2,4 - 3,0	3,5	0,3
Cr	16	9 - 23	19	3
Cu	11,4	9,1 - 13,6	14,2	1,8
Dy	0,40	0,30 - 0,50	0,59	0,16
Eu	0,37	0,28 - 0,46	0,51	0,13
Fe	29	21 - 37	40	8
Gd	0,24	0,13 - 0,35	0,90	0,38
In	2,5	1,7 - 3,3	4,7	0,7
K	48	43 - 53	46	12
Li	3,25	2,60 - 3,90	3,73	0,44
Mg	5,4	4,6 - 6,2	8,8	2,2
Mn	5,73	4,9 - 6,6	7,24	1,32
Mo	5,3	4,5 - 6,2	6,7	0,9
Ni	23,2	20,7 - 25,7	25,0	2,5
Sb	1,6	1,2 - 2,0	4,2	0,7
Si	13	8 - 19	31	8
Sm	0,41	0,35 - 0,47	0,59	0,10
Th	-	-	1,1	0,2
Ti	5,5	4,2 - 6,9	6,3	1,1
V	0,44	0,29 - 0,59	0,79	0,17
W	2,8	2,4 - 3,2	3,3	1,5
Zn	22,9	18,9 - 26,8	29,0	4,0
Zr	40		37	3,4

Table 6.7: Comparison of U_3O_8-Standard ES 5 with SSMS

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error of 95% CL
Al	12	0 - 15	14	3,4
B	0,4	0,30 - 0,40	0,9	0,2
Bi	0,6	0,5 - 0,8	1,6	0,6
Ca	11	9,7 - 12,3	29	6,7
Cd	0,1	-	0,64	0,2
Co	2,6	2,3 - 2,9	3,8	0,5
Cr	12	7 - 17	12	2
Cu	6,2	5,0 - 7,5	8,5	0,8
Dy	0,23	0,16 - 0,30	0,50	0,38
Eu	0,22	0,16 - 0,28	0,36	0,08
Fe	19	13 - 25	24	5
Gd	0,16	0,08 - 0,20	0,39	0,02
In	1,8	1,2 - 2,4	3,1	0,5
K	20	17 - 22	22	7
Li	1,86	1,47 - 2,25	2,37	0,86
Mg	2,4	2,0 - 2,8	5,9	1,7
Mn	3,09	2,6 - 3,6	4,8	0,9
Mo	20,9	17,6 - 24,2	24,4	2,6
Ni	12,8	11,4 - 14,2	15,4	2,0
Sb	0,5	0,3 - 0,8	2,6	0,6
Si	-	-	85	33
Sm	0,18	0,14 - 0,22	0,30	0,26
Th	-	-	0,71	0,2
Ti	3,1	2,3 - 3,9	4,5	0,8
V	0,14	0,05 - 0,23	0,39	0,1
W	0,9	0,8 - 1,1	1,2	1,0
Zn	13,2	10,8 - 15,6	18,1	3,3
Zr	27	-	23	2

CHAPTER SEVEN

GENERAL COMMENTS AND CONCLUSIONS

The success of the project for the development of analytical and data interpretation methods for the qualitative and quantitative analysis of trace impurities in uranium compounds with spark-source mass spectrometry has been adequately demonstrated.

Not only did the mass spectrometry results contribute to the characterisation of the internal U_3O_8 impurity standards, but the analytical data was in many cases closer to the expected values than those of any of the other analytical techniques.

Furthermore, the ability to analyse UF_4 materials provided analytical results which could not be obtained with any other technique available at the time.

The use of the ratio between singly and doubly charged exposure values as well as the use of the mean exposure value for the internal standard to determine whether a photoplate is acceptable or not, is a new approach to data interpretation in spark-source mass spectrometry. In this way possible misleading results can be directly avoided. Other quality assurance data interpretation methods have also been introduced. This thesis is now being used as a reference document for the mass spectrometry laboratory.

Contamination is an ever present threat to elemental trace level analysis. An effective but expensive solution would be a laboratory conforming to class 100 requirements. A relatively inexpensive alternative has been implemented in this laboratory. A laminar flow cabinet, where a curtain of HEPA filtered air is induced at the opening, is used for all sample preparation steps. Due to the positive pressure of air within the cabinet no contamination in the form of dust can enter.

The apparent disadvantages of the spark-source mass spectrometric technique are:

1 Successful use requires wide experience, both in the operation of equipment and in the reading and interpretation of spectra.

2 The instrument is essentially a comparator; for quantitative analyses, standards of composition similar to the material under analysis are required. Unknown samples therefore present a problem when quantitative results are required.

3 The accuracy and precision are not as high as for some spectroscopic methods, notably inductively coupled plasma mass spectrometry (ICP-MS). It should be realised that these techniques have their own unique limitations, for example, laser ablation has a big problem with point inhomogeneity.

The use of spark-source mass spectrometry to analyse trace impurities in uranium compounds is still one of the most powerful techniques available. This is confirmed by the following advantages:

1 The procedure is specific for the element being determined. Sources of interference can be unequivocally identified and in many cases eliminated.

2 Quantitative determination of traces of the elements in a powder sample can be achieved without any preliminary chemical treatment. All solid materials may be determined.

3 A permanent record is obtained on a photographic plate.

4 *The technique may be applied to the determination of small quantities of added constituents or of traces of impurities to solid-state matrices where conventional methods of analysis are difficult, fail, or give less accurate results.*

5 *The information content of analytical data which can be utilised is vast. This compensates for the relatively high operation costs of the technique. A direct complete picture can be obtained for all major and minor elements with the analysis of a single sample. This is especially useful when characterising unknown samples as well as for semi-quantitative analyses. Quantitative analysis with alternative methods for the identified impurities can then be executed cost effectively.*

6 *All isotopes of an element are recorded on a photoplate with intensities according to their isotopic abundances which leads to undisputed confirmation that a particular element is present in the sample as an impurity.*

7 *The up-time and reliability of the instrument is a proven fact, making this technique comparable if not better than any other analytical technique in this field.*

Spark-source mass spectrometry today has wider applications than just for the analysis of uranium compounds. Fields in which this technique is actively used include biomedical [42], geological [43] and horticultural science [44], as well as agricultural and environmental sciences [45]. It continues to play a prominent role in the contemporary nuclear technology laboratory [46, 47].

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APPENDIX A

LINEAR REGRESSION FORMULAE [29]

$y = mx + c$

$$m = \frac{(n\sum_{j=1}^{n} x_j y_j) - [(\sum_{j=1}^{n} x_j)(\sum_{j=1}^{n} y_j)]}{(n\sum_{j=1}^{n} x_j^2) - (\sum_{j=1}^{n} x_j)^2}$$

$$s = \left(\frac{s_{yy} - m\, s_{xy}}{n-2}\right)^{1/2}$$

$$s_{yy} = (\sum_{j=1}^{n} y_j^2) - \frac{(\sum_{j=1}^{n} y_j)^2}{n}$$

$$s_{xx} = (\sum_{j=1}^{n} x_j^2) - \frac{(\sum_{j=1}^{n} x_j)^2}{n}$$

$$s_{xy} = (\sum_{j=1}^{n} x_j y_j) - \frac{(\sum_{j=1}^{n} x_j)(\sum_{j=1}^{n} y_j)}{n}$$

$$c = \left(\frac{\sum_{j=1}^{n} y_j}{n}\right) - m\left(\frac{\sum_{j=1}^{n} x_j}{n}\right)$$

$$s_m = \frac{s}{(s_{xx})^{1/2}}$$

$$s_c = \frac{s(\sum_{j=1}^{n} x_j^2)^{1/2}}{(n\, s_{xx})^{1/2}}$$

APPENDIX B

TABLE OF ATOMIC AND MOLECULAR LINES FOR SPARK SOURCE MASS SPECTROMETRY OF COMPLEX SAMPLE-GRAPHITE MIXES

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ABSTRACT

A detailed table of atomic and molecular mass spectral lines has been prepared to aid in the interpretation of interferences and assignment of spectral lines in complex spectra arising from the spark source analysis of natural insulating powders blended with graphite to sustain the RF spark. The compilation consisting of 3000 listings is particularly useful for multielement trace analysis of geological and biological solids. Included are carbides, oxides, polymers, multiply-charged ions, and other molecular species of several or more major and minor elements as well as a large number of trace elements.

INTRODUCTION

Spark source mass spectrometry is a useful technique for multielemental trace analysis of geological and biological solids. Such insulating materials are usually powdered and mixed with graphite to produce strong and conducting electrodes. However, the sparking of complex graphite mixes yields complicated spectra containing the carbides, oxides, polymers, multiply-charged ions, and other molecular species of several or more major and minor elements as well as a large number of trace elements.

The primary purpose of the following table is to aid in the interpretation of interferences and assignment of spectral lines in complex spectra arising from the spark source analysis of natural insulating powders in a graphite matrix. In a secondary sense, the table may also be applied to other sample types or even to other fields of mass spectrometry such as ion probe analysis where molecular species become relatively more important.

There are indeed other excellent mass tables available for general use, but they are limited for application to the specific problem as stated. More explicitly, the table of Owens and Sherman (1) is arranged by individual element with comprehensive coverage for certain kinds of species excluding carbides, oxides, and many molecular species. The table of Guthrie and Heath (2), albeit arranged by mass, excludes carbides, most oxides, charge-exchange species, and other species of interest. The aim herein is to include those species omitted in preceding tables but of possible interest in complex graphite systems, to arrange the table in order of ascending mass values, to include the relative abundance of each species listed, to indicate the theoretical resolution required to separate a listed species from a line of analytical value, and finally to be concise in format but comprehensive in scope. The latter requirement,has resulted in approximately 3000 listings each containing four data words and producing a text of approximately 12,000 words on a physical format of only thirteen pages.

The entire table was manually calculated, compiled, and typed and is therefore not meant as a manual of supercritical mass and abundance data, but merely as an interpretive and useful guide. The user must assume any liability of any kind incurred in the employment of this table. Further, no claim is made as to the existence or nonexistence of any species listed herein, nor to that of any species accidentally or purposely omitted.

EXPLANATION OF TABLE

Each listing consists of a row of four words starting with the name of the species and followed by the mass, abundance, and resolutional requirement of the named species respectively.

I. NOMENCLATURE OF SPECIES

The usual chemical notation is used to identify the elemental constuents of the species. A leading superscript refers to the nominal mass of the species and a trailing superscript refers to the positive charge of the species. The plus signs of the charge superscripts are omitted since all species are ions of positive charge. The charge superscript is omitted entirely for species having a single positive charge. A special two-digit charge superscript indicates a charge-exchange species where the first digit is the initial charge of the species before a charge-reducing collision and the second digit gives the resulting or final charge after collision. The general nomenclature and the special meaning of the nominal mass superscript are best illustrated by example.

I.A. Elementally Homogeneous Species

(a) ^{12}C : a singly-charged ion of carbon 12
(b) $^{12}C^{3}$: a triply-charged ion of carbon 12
(c) $^{12}C_2$: a homo-isotopic dimer of carbon and the only combination of carbon isotopes having a nominal mass of 24. (Absence of superscript = +1).
(d) $^{25}C_2^2$: a hetero-isotopic dimer of carbon having a +2 positive charge and containing all combinations of carbon isotopes having a nominal mass of 25. (Only one combination in this case).
(e) $^{86}Si_3$: a trimer of silicon containing all combinations of silicon isotopes giving a nominal mass of 86, ie, $^{86}Si_3 = (^{28}Si_2 + ^{30}Si) + (^{28}Si + ^{29}Si_2)$, where the parentheses indicate the combinations having the same nominal mass.
(f) $^{12}C^{32}$: a charge-exchange species of carbon 12 where the initial charge is +3 and the final charge is +2.

I.B. Elementally Heterogeneous Species

(a) ^{28}SiC : a monocarbide of silicon 28 and the only significant* combination of carbon and silicon isotopes having a nominal mass of 40.
(b) ^{41}SiC : all the combinations** of silicon and carbon isotopes having a nominal mass of 41, ie, $(^{29}Si + ^{12}C)$ and $(^{28}Si + ^{13}C)$.
(c) $^{28}Si_3C_2$: the only significant* combination of silicon and carbon isotopes having a nominal mass of 108, ie, there is only one silicon trimer of nominal mass 84 and only one carbon dimer of nominal mass 24.
(d) $^{109}Si_3C_2$: all the combinations** of silicon trimer and carbon dimer having a nominal mass of 109, ie, $(^{85}Si_3 + ^{12}C_2)$ and $(^{28}Si_3 + ^{25}C_2)$.

* The word 'significant' means that if a single combination of isotopes is cited, then it is either the only possible combination or a combination which accounts for 99.0% or more of the abundance of all possible combinations.

** The phrase 'all the combinations' means that the combinations included are either the only possible ones or that they cumulatively account for 99.0% or more of the abundance of all combinations.

The starred definitions have meaning in relation to the mass and abundance data following a cited species (see parts II and III).

II. MASS (second word)

The masses of singly-charged species are taken from the table of Guthrie and Heath (2) and are rounded to five decimal places. Some elements are known to less than five places while others are only approximated as indicated by a (/) following the last digit in the mass value. Polymeric and heterogeneous species have masses equal to the sum of the individual contributing masses. Charge-exchange masses are obtained by multiplying the singly-charged mass by a factor (m/n^2) where (m) is the initial and (n) the final charge of the ion. Multiply-charged ions have masses equal to the singly-charged mass divided by the integral number of positive charges.

For species containing more than one combination of isotopes (eg., I.A.e, I.B.b, and I.B.d), the mass is that of the combination of isotopes which is the most abundant, as opposed to masses of single combinations which are unequivocal. The grouping of combinations of isotopes of the same elements to produce a species of the same chemical formula was performed to reduce the number of listings and is based on the fact that the combinations in a group are not resolvable with present commercial apparatus which have resolutions of 10,000 maximum and 5,000 or less practical.

III. ABUNDANCE (third word)

Isotopic abundances are based on Guthrie and Heath (2). Abundances apply only to species of the same kind (same chemical formula, same charge, but possibly different exact masses). For example, ^{28}SiC at mass 39.97693 comprises 91.19% of the total amount of silicon carbide formed from all combinations of silicon and carbon isotopes, ^{41}SiC at mass 40.97649 accounts for 5.67%, etc. The abundance of ^{28}SiC is that of a single combination while that of ^{41}SiC is the sum of the abundances of more than one combination.

The abundances of molecular species which are elementally homogeneous are calculated using the binomial expansion according to Hill (3) or the equivalent probability formula given by Owens and Sherman (1) for polyatomic clusters:

$$RA = (A^a B^b C^c \ldots N^n)(M!)/(a!b!c!..n!) \qquad 1.$$

where RA is the relative abundance of a given polyatomic cluster (a specified combination of isotopes) containing M total atoms of an element which has isotopes A', B', C',....N' with isotopic abundances A, B, C, ...N respectively and where the number of atoms of each isotope contained in the cluster is a, b, c, ...n respectively. The summation (a+b+c+...n) is equal to M. This formula is applied to each specific combination of isotopes until all possible combinations are exhausted.

For clusters containing different elements, the above formula is applied to each element individually and the abundance of the heterogeneous cluster is taken as the product of the indivual RA's for each element in the cluster.

The tabled abundances are given in percent. The appearance of an (E) in the tabled abundance indicates a negative exponential form so that 1.2E3, for example, means 00.0012%.

For species containing more than one combination (seeI), the abundance is the sum of all combinations considered, whereas the mass is that of the most abundant combination.

IV. RESOLUTIONAL REQUIREMENT (fourth word)

Resolution is defined as $R = M_0/\Delta M$. M_0 is indicated in the table by a series of five dashes for a line of interest at each nominal mass unit and at some half-mass units where appropriate. A negative value for R indicates that the listed species occurs at a lower mass than M_0, the latter being indicated by the next dashed line. A positive value of R indicates a higher mass than M_0 which is defined as the first previous dashed line.

The appearance of an (E) in the resolution value indicates a positive exponential form so that 15E3, for example, means a resolution of 15,000. There are no exponential forms for resolutions less than 10,000 (= 10E3).

V. SCOPE

The number and kinds of species included for each element depends on its definition as a major, minor, or trace constituent in geological and biological samples. Carbon, being the matrix considered, is defined as a major element. Other defined majors are oxygen, sodium, silicon, phosphorous, sulfur, potassium, calcium, titanium, and iron. Minors are given as chromium, nickel, zinc, strontium, zirconium, and barium. Most other elements are defined as trace.

For trace elements the species considered are: singly-and-multiply charged ions up to +3, polymerization up to the dimer only, mono-and-dicarbides, and mono-and-di-oxides.

For minor elements the species are: singly-and-multiply charged ions up to +4, polymerization up to the trimer, formation of oxide up to the trioxide and carbide to the tricarbide, and charge-exchange species with initial charges of +4 or less.

Major elements have more extensive coverage: singly-and-multiply charged ion up to +6, polymerization up to four atoms, formation of tetra-oxide and tetra-carbide, charge-exchange species with initial charge of 7 or less, and some complex species having two atoms of the major species and one to three atoms or carbon or oxygen. Polymer formers such as carbon, aluminum, and silicon are considered to form even more complex species and some combinations of these elements with other major elements are included. Appropriate higher degrees of polymerization and carbide and oxide formation are listed for these three elements.

Only the lower-charged species of rare gases are considered.

Hydrocarbons up to mass 100 are included.

The first hydrides(MH) of all elements from lithium to molybdenum plus barium, lanthanum, and cerium are also listed.

The mass range covered is from 1 to 270 with reductions in the number of entries from mass 210 to 270 where only two elements, thorium and uranium, are of interest.

REFERNCES

1. E.B. Owens and A.M. Sherman, Mass Spectrographic Lines of the Elements, MIT Tech. Rep. No. 265, 1962
2. J.W. Guthrie and R.L. Heath, Table of Atomic Masses, Sandia Corporation Monograph SCR-245, 16th Ed., 1961
3. H.C. Hill, Introduction to Mass Spectrometry, Heydon and Son, London, 1966

$^{1}\mathrm{H}$	1.00782	99.985	
$^{3}\mathrm{He}^{2}$	1.50801	01.4E4	
$^{12}\mathrm{C}^{6}$	2.00000	98.893	- 143
$^{4}\mathrm{He}^{2}$	2.00130	99.999	- 157
$^{6}\mathrm{Li}^{3}$	2.00500	07.42	- 221
$^{2}\mathrm{D}$	2.01410	00.015	-----
$^{1}\mathrm{H}_{2}$	2.01565	99.970	+1300
$^{13}\mathrm{C}^{6}$	2.16723	01.107	
$^{12}\mathrm{C}^{7\,6}$	2.33328	99.893	
$^{7}\mathrm{Li}^{3}$	2.33870	92.58	
$^{13}\mathrm{C}^{7\,6}$	2.52837	01.107	
$^{13}\mathrm{C}^{5}$	2.60067	01.107	
$^{16}\mathrm{O}^{6}$	2.66582	99.759	
$^{14}\mathrm{N}^{5}$	2.80061	99.634	
$^{17}\mathrm{O}^{6}$	2.83319	00.037	
$^{12}\mathrm{C}^{65}$	2.88000	98.893	
$^{18}\mathrm{O}^{6}$	2.99986	00.204	- 186
$^{12}\mathrm{C}^{4}$	3.00000	98.893	- 187
$^{9}\mathrm{Be}^{3}$	3.00407	100.000	- 252
$^{6}\mathrm{Li}^{2}$	3.00756	07.42	- 356
$^{3}\mathrm{He}$	3.01603	01.4E4	-----
$^{3}\mathrm{H}$	3.01605	....	+15E4
$^{3}\mathrm{H}_{2}$	3.02193	00.030	+ 512
$^{16}\mathrm{O}^{7\,6}$	3.11051	99.759	
$^{13}\mathrm{C}^{65}$	3.12080	01.107	
$^{16}\mathrm{O}^{5}$	3.19898	99.759	
$^{13}\mathrm{C}^{4}$	3.25084	01.107	
$^{17}\mathrm{O}^{7\,6}$	3.30531	00.037	
$^{10}\mathrm{Be}^{3}$	3.33765	19.61	
$^{17}\mathrm{O}^{5}$	3.39982	00.037	
$^{18}\mathrm{O}^{7\,6}$	3.49976	00.204	- 437
$^{14}\mathrm{N}^{4}$	3.50077	99.634	- 485
$^{7}\mathrm{Li}^{2}$	3.50800	92.58	-----
$^{18}\mathrm{O}^{5}$	3.59983	00.204	
$^{11}\mathrm{B}^{3}$	3.66977	80.39	
$^{12}\mathrm{C}^{54}$	3.75000	98.893	
$^{15}\mathrm{N}^{4}$	3.75003	00.366	
$^{23}\mathrm{Na}^{6}$	3.83163	100.000	
$^{16}\mathrm{O}^{65}$	3.83878	99.759	
$^{24}\mathrm{Mg}^{6}$	3.99751	78.70	- 786
$^{16}\mathrm{O}^{4}$	3.99873	99.759	-1034
$^{12}\mathrm{C}^{3}$	4.00000	98.893	-1540
$^{4}\mathrm{He}$	4.00260	99.999	-----
$^{2}\mathrm{H}_{2}$	4.02820	02.0E4	+ 156
$^{13}\mathrm{C}^{54}$	4.06355	01.107	
$^{17}\mathrm{O}^{65}$	4.07979	00.037	
$^{25}\mathrm{Mg}^{6}$	4.16431	10.13	
$^{17}\mathrm{O}^{4}$	4.24978	00.037	
$^{18}\mathrm{O}^{65}$	4.31980	00.204	
$^{26}\mathrm{Mg}^{6}$	4.33043	11.17	- 829
$^{13}\mathrm{C}^{3}$	4.33445	01.107	-----
$^{14}\mathrm{N}^{54}$	4.37596	99.634	
$^{27}\mathrm{Al}^{6}$	4.49692	100.000	-1570
$^{18}\mathrm{O}^{4}$	4.49979	00.204	-----
$^{9}\mathrm{Be}^{2}$	4.50610	100.000	+ 713
$^{23}\mathrm{Na}^{5}$	4.59796	100.000	
$^{28}\mathrm{Si}^{6}$	4.66282	92.21	- 960
$^{14}\mathrm{N}^{3}$	4.66769	99.634	-----
$^{19}\mathrm{F}^{4}$	4.74960	100.000	
$^{24}\mathrm{Mg}^{5}$	4.79717	78.70	
$^{29}\mathrm{Si}^{6}$	4.82941	04.70	
$^{30}\mathrm{Si}^{6}$	4.99563	03.09	-----
$^{25}\mathrm{Mg}^{5}$	4.99717	10.13	+3240
$^{16}\mathrm{O}^{54}$	4.99841	99.759	+1797
$^{15}\mathrm{N}^{3}$	5.00004	00.366	+1130
$^{10}\mathrm{B}^{2}$	5.00647	19.61	+ 461
$^{31}\mathrm{P}^{6}$	5.16229	100.000	
$^{26}\mathrm{Mg}^{5}$	5.19652	11.17	
$^{17}\mathrm{O}^{54}$	5.31223	00.037	- 275
$^{32}\mathrm{S}^{6}$	5.32868	95.0	-1801
$^{16}\mathrm{O}^{3}$	5.33164	99.759	-----
$^{12}\mathrm{C}^{43}$	5.33333	98.893	+3149
$^{33}\mathrm{S}^{6}$	5.49524	00.76	- 585
$^{11}\mathrm{B}^{2}$	5.50465	80.39	-----
$^{28}\mathrm{Si}^{5}$	5.59539	92.21	
$^{18}\mathrm{O}^{54}$	5.62474	00.204	
$^{34}\mathrm{S}^{6}$	5.66131	04.22	-1120
$^{17}\mathrm{O}^{3}$	5.66638	00.037	-----
$^{23}\mathrm{Na}^{4}$	5.74745	100.000	-----
$^{24}\mathrm{Mg}^{65}$	5.75641	78.70	+ 642
$^{13}\mathrm{C}^{43}$	5.77926	01.107	+ 181
$^{28}\mathrm{Si}^{5}$	5.79530	04.70	
$^{36}\mathrm{S}^{6}$	5.99451	00.014	- 292
$^{36}\mathrm{A}^{6}$	5.99459	00.337	- 293
$^{30}\mathrm{Si}^{5}$	5.99475	03.09	- 295
$^{24}\mathrm{Mg}^{4}$	5.99626	78.70	- 319
$^{25}\mathrm{Mg}^{65}$	5.99660	10.13	- 327
$^{18}\mathrm{O}^{3}$	5.99972	00.204	- 391
$^{12}\mathrm{C}^{2}$	6.00000	98.893	- 398
$^{6}\mathrm{Li}$	6.01512	07.42	-----
$^{31}\mathrm{P}^{5}$	6.19476	100.000	
$^{14}\mathrm{N}^{43}$	6.22358	99.634	- 273
$^{26}\mathrm{Mg}^{65}$	6.23582	11.17	- 587
$^{25}\mathrm{Mg}^{4}$	6.24646	10.13	-----
$^{19}\mathrm{F}^{3}$	6.33280	100.000	
$^{32}\mathrm{S}^{5}$	6.39441	95.0	
$^{27}\mathrm{Al}^{65}$	6.47557	100.000	- 323
$^{39}\mathrm{K}^{6}$	6.49395	93.10	-3820
$^{26}\mathrm{Mg}^{4}$	6.49565	11.17	-----
$^{13}\mathrm{C}^{2}$	6.50168	01.107	+1077
$^{33}\mathrm{S}^{5}$	6.59429	00.76	
$^{40}\mathrm{A}^{6}$	6.66040	99.6	-22E4
$^{40}\mathrm{Ca}^{6}$	6.66043	96.97	-----
$^{40}\mathrm{K}^{6}$	6.66067	00.012	+27E3
$^{20}\mathrm{Ne}^{3}$	6.66415	90.92	+1790
$^{12}\mathrm{C}^{53}$	6.66666	98.893	+1064
$^{28}\mathrm{Si}^{65}$	6.71446	92.21	
$^{27}\mathrm{Al}^{4}$	6.74538	100.000	
$^{34}\mathrm{S}^{5}$	6.79358	100.000	
$^{41}\mathrm{K}^{6}$	6.82697	06.88	
$^{29}\mathrm{Si}^{65}$	6.95436	04.70	
$^{42}\mathrm{Ca}^{6}$	6.99310	00.64	- 306
$^{35}\mathrm{Cl}^{5}$	6.99377	75.529	- 316
$^{28}\mathrm{Si}^{4}$	6.99423	92.21	- 322
$^{21}\mathrm{Ne}^{3}$	6.99795	00.257	- 389
$^{14}\mathrm{N}^{2}$	7.00154	99.638	- 485
$^{7}\mathrm{Li}$	7.01600	92.58	-----
$^{6}\mathrm{LiH}$	7.02282	07.42	+1029
$^{16}\mathrm{O}^{43}$	7.10885	99.759	
$^{43}\mathrm{Ca}^{6}$	7.15980	00.146	
$^{23}\mathrm{Na}^{54}$	7.18431	100.000	-----
$^{30}\mathrm{Si}^{65}$	7.19370	03.09	+ 765
$^{36}\mathrm{S}^{5}$	7.19342	00.014	+ 789
$^{36}\mathrm{A}^{5}$	7.19351	00.337	+ 781
$^{13}\mathrm{C}^{53}$	7.22409	01.107	
$^{29}\mathrm{Si}^{4}$	7.24412	04.70	
$^{44}\mathrm{Ca}^{6}$	7.32592	02.06	-----
$^{22}\mathrm{Ne}^{3}$	7.33046	08.82	+1614
$^{37}\mathrm{Cl}^{5}$	7.39318	24.471	
$^{31}\mathrm{P}^{65}$	7.43370	100.000	
$^{45}\mathrm{Sc}^{6}$	7.49265	100.000	-9490
$^{30}\mathrm{Si}^{4}$	7.49344	03.09	-----
$^{24}\mathrm{Mg}^{54}$	7.49533	78.70	+3965
$^{15}\mathrm{N}^{2}$	7.50005	00.366	+1134
$^{17}\mathrm{O}^{43}$	7.55170	00.037	
$^{32}\mathrm{S}^{65}$	7.67330	95.0	
$^{31}\mathrm{P}^{4}$	7.74344	100.000	
$^{39}\mathrm{K}^{5}$	7.79274	93.10	-----
$^{25}\mathrm{Mg}^{54}$	7.80807	10.13	+ 508
$^{47}\mathrm{Ti}^{6}$	7.82529	07.29	+ 240
$^{48}\mathrm{Ti}^{6}$	7.99132	73.98	-1303
$^{48}\mathrm{Ca}^{6}$	7.99209	00.185	-1489
$^{40}\mathrm{A}^{5}$	7.99248	99.6	-1606
$^{40}\mathrm{Ca}^{5}$	7.99252	96.97	-1619
$^{40}\mathrm{K}^{5}$	7.99280	00.012	-1717
$^{32}\mathrm{S}^{4}$	7.99302	95.0	-1801
$^{24}\mathrm{Mg}^{3}$	7.99501	78.70	-3264
$^{16}\mathrm{O}^{2}$	7.99746	99.759	-----
$^{18}\mathrm{O}^{43}$	7.99963	00.204	+3685
$^{7}\mathrm{LiH}$	8.02382	92.57	+ 303
$^{26}\mathrm{Mg}^{54}$	8.11956	11.17	
$^{34}\mathrm{S}^{65}$	8.15229	04.22	-1434
$^{49}\mathrm{Ti}^{6}$	8.15798	05.51	-----
$^{41}\mathrm{K}^{5}$	8.19237	06.88	
$^{33}\mathrm{S}^{4}$	8.24287	00.76	
$^{50}\mathrm{Ti}^{6}$	8.24287	05.34	-1847
$^{50}\mathrm{Cr}^{6}$	8.32434	04.31	-1950
$^{50}\mathrm{V}^{6}$	8.32453	00.24	-2040
$^{25}\mathrm{Mg}^{3}$	8.32861	10.13	-----
$^{42}\mathrm{Ca}^{5}$	8.39173	00.64	+ 132
$^{27}\mathrm{Al}^{54}$	8.43173	100.00	-----
$^{19}\mathrm{F}^{43}$	8.44373	100.00	+ 703
$^{51}\mathrm{V}^{6}$	8.49066	99.76	- 954
$^{34}\mathrm{S}^{4}$	8.49197	04.22	-1118
$^{17}\mathrm{O}^{2}$	8.49957	00.037	-----
$^{43}\mathrm{Ca}^{5}$	8.59176	00.146	
$^{52}\mathrm{Cr}^{6}$	8.65675	83.76	-2107
$^{26}\mathrm{Mg}^{3}$	8.66086	11.17	-----
$^{35}\mathrm{Cl}^{4}$	8.74221	75.529	-----
$^{28}\mathrm{Si}^{54}$	8.75279	92.21	+ 826
$^{44}\mathrm{Ca}^{5}$	8.79110	02.06	
$^{53}\mathrm{Cr}^{6}$	8.82344	09.55	
$^{16}\mathrm{O}^{53}$	8.88606	99.759	
$^{54}\mathrm{Cr}^{6}$	8.98981	02.38	- 403
$^{54}\mathrm{Fe}^{6}$	8.98993	05.82	- 405
$^{45}\mathrm{Sc}^{5}$	8.99118	100.000	- 429
$^{36}\mathrm{S}^{4}$	8.99177	00.014	- 441
$^{36}\mathrm{A}^{4}$	8.99189	00.337	- 444
$^{27}\mathrm{Al}^{3}$	8.99384	100.000	- 491
$^{18}\mathrm{O}^{2}$	8.99958	00.204	- 714
$^{12}\mathrm{C}^{32}$	9.00000	98.893	- 739
$^{9}\mathrm{Be}$	9.01219	100.000	-----
$^{29}\mathrm{Si}^{54}$	9.05515	04.70	+ 210
$^{55}\mathrm{Mn}^{6}$	9.15634	100.000	
$^{46}\mathrm{Ti}^{5}$	9.19053	08.00	-----
$^{46}\mathrm{Ca}^{5}$	9.19074	00.003	+44E3
$^{37}\mathrm{Cl}^{4}$	9.24148	24.471	
$^{56}\mathrm{Fe}^{6}$	9.32249	91.66	-2961
$^{28}\mathrm{Si}^{3}$	9.32564	92.21	-----
$^{39}\mathrm{K}^{65}$	9.35129	93.10	- 604
$^{30}\mathrm{Si}^{54}$	9.36680	03.09	-----
$^{47}\mathrm{Ti}^{5}$	9.39075	07.29	
$^{17}\mathrm{O}^{53}$	9.44396	00.037	
$^{57}\mathrm{Fe}^{6}$	9.48923	02.19	- 953
$^{38}\mathrm{A}^{4}$	9.49068	00.063	-1115
$^{19}\mathrm{F}^{2}$	9.49920	100.000	-----
$^{48}\mathrm{Ti}^{5}$	9.58959	73.98	-----
$^{48}\mathrm{Ca}^{5}$	9.59051	00.185	+10E3
$^{44}\mathrm{Ca}^{65}$	9.59102	02.06	+6706
$^{58}\mathrm{Fe}^{6}$	9.65555	00.33	-2945
$^{58}\mathrm{Ni}^{6}$	9.65589	69.18	-3285
$^{29}\mathrm{Si}^{3}$	9.65883	04.70	-----
$^{31}\mathrm{P}^{54}$	9.67930	100.00	+ 472
$^{39}\mathrm{K}^{4}$	9.74093	93.10	-----
$^{13}\mathrm{C}^{32}$	9.75252	01.107	+ 840
$^{49}\mathrm{Ti}^{5}$	9.78957	05.51	
$^{59}\mathrm{Co}^{6}$	9.82221	100.000	-----
$^{41}\mathrm{K}^{65}$	9.83084	93.10	+1138
$^{60}\mathrm{Ni}^{6}$	9.98846	26.23	- 409
$^{50}\mathrm{Ti}^{5}$	9.98896	05.34	- 418
$^{50}\mathrm{Cr}^{5}$	9.98921	04.31	- 422
$^{50}\mathrm{V}^{5}$	9.98943	00.24	- 426
$^{32}\mathrm{S}^{54}$	9.99127	95.0	- 462
$^{20}\mathrm{Ne}^{2}$	9.99622	90.92	- 599
$^{18}\mathrm{O}^{53}$	9.99953	00.204	- 747
$^{10}\mathrm{B}$	10.01294	19.61	-----
$^{10}\mathrm{Be}$	10.01354	-----	+17E3
$^{9}\mathrm{BeH}$	10.02001	99.985	+1416
$^{61}\mathrm{Ni}^{6}$	10.15518	01.19	
$^{51}\mathrm{V}^{5}$	10.18880	99.76	
$^{23}\mathrm{Na}^{43}$	10.21767	100.000	
$^{41}\mathrm{K}^{4}$	10.24046	06.88	
$^{62}\mathrm{Ni}^{6}$	10.32139	03.66	-3226
$^{31}\mathrm{P}^{3}$	10.32459	100.00	-----
$^{52}\mathrm{Cr}^{6}$	10.38810	83.76	
$^{63}\mathrm{Cu}^{6}$	10.48827	60.09	-7547
$^{42}\mathrm{Ca}^{4}$	10.48966	00.64	-----
$^{21}\mathrm{Ne}^{2}$	10.49692	00.257	+1445
$^{14}\mathrm{N}^{32}$	10.50231	99.634	+ 829
$^{44}\mathrm{Ca}^{65}$	10.54932	02.06	
$^{53}\mathrm{Cr}^{5}$	10.58813	09.55	
$^{34}\mathrm{S}^{54}$	10.61496	04.22	
$^{64}\mathrm{Ni}^{6}$	10.65466	01.08	-3947
$^{64}\mathrm{Zn}^{6}$	10.65486	48.89	-4263
$^{32}\mathrm{S}^{3}$	10.65736	95.0	-----
$^{24}\mathrm{Mg}^{43}$	10.66002	78.70	+1702
$^{43}\mathrm{Ca}^{4}$	10.73970	00.146	- 224
$^{54}\mathrm{Cr}^{5}$	10.78777	02.38	-72E3
$^{54}\mathrm{Fe}^{5}$	10.78792	05.82	-----
$^{65}\mathrm{Cu}^{6}$	10.82130	30.91	+ 323
$^{55}\mathrm{Mn}^{5}$	10.98761	100.00	- 507
$^{66}\mathrm{Zn}^{6}$	10.98768	27.81	- 509
$^{44}\mathrm{Ca}^{4}$	10.98887	02.06	- 539
$^{33}\mathrm{S}^{3}$	10.99049	00.76	- 585
$^{22}\mathrm{Ne}^{2}$	10.99569	08.82	- 808
$^{11}\mathrm{B}$	11.00931	80.39	-----
$^{10}\mathrm{BH}$	11.02076	19.61	+ 962
$^{46}\mathrm{Ti}^{65}$	11.02863	08.00	+ 570

$^{25}Mg^{43}$	11.10482	10.13	
$^{67}Zn^{6}$	11.15452	04.11	- 344
$^{56}Fe^{5}$	11.18699	91.66	-----
$^{45}Sc^{4}$	11.23898	100.00	
$^{47}Ti^{65}$	11.26842	07.29	
$^{68}Zn^{6}$	11.32081	18.57	-6256
$^{34}S^{3}$	11.32262	04.22	-----
$^{57}Fe^{5}$	11.38703	02.19	
$^{69}Ga^{6}$	11.48762	60.4	-1581
$^{46}Ti^{4}$	11.48816	08.00	-1708
$^{46}Ca^{4}$	11.48842	00.003	-1777
$^{23}Na^{2}$	11.49489	100.000	-----
$^{48}Ti^{65}$	11.50751	73.98	+ 911
$^{26}Mg^{43}$	11.54782	11.17	
$^{58}Fe^{5}$	11.58666	00.33	-28E3
$^{58}Ni^{5}$	11.58707	69.18	-----
$^{70}Ge^{6}$	11.65400	20.52	-5112
$^{70}Zn^{6}$	11.65422	00.62	-5658
$^{35}Cl^{3}$	11.65628	75.529	-----
$^{47}Ti^{4}$	11.73794	07.29	
$^{59}Co^{5}$	11.78664	100.00	
$^{71}Ga^{6}$	11.82080	39.6	
$^{60}Ni^{5}$	11.98615	26.23	- 866
$^{50}Ti^{65}$	11.98675	05.45	- 906
$^{72}Ge^{6}$	11.98693	27.43	- 918
$^{48}Ti^{4}$	11.98699	73.98	- 922
$^{50}Cr^{65}$	11.98705	04.31	- 927
$^{48}Ca^{4}$	11.98813	00.185	-1011
$^{36}S^{3}$	11.98903	00.014	-1094
$^{36}A^{3}$	11.98913	00.337	-1110
$^{27}Al^{43}$	11.99180	100.00	-1463
$^{24}Mg^{2}$	11.99252	78.70	-1604
$^{16}O^{32}$	11.99619	99.759	-3150
^{12}C	12.00000	98.893	-----
^{11}BH	12.01713	80.38	+ 701
$^{6}Li_2$	12.03000	00.551	+ 400
$^{73}Ge^{6}$	12.15389	07.76	- 547
$^{39}K^{54}$	12.17616	93.10	-----
$^{61}Ni^{5}$	12.18622	01.19	+1210
$^{49}Ti^{4}$	12.23697	05.51	
$^{74}Ge^{6}$	12.32017	36.54	-6845
$^{74}Se^{6}$	12.32042	00.87	-7950
$^{37}Cl^{3}$	12.32197	24.471	-----
$^{62}Ni^{5}$	12.38567	03.66	
$^{28}Si^{43}$	12.43418	92.21	
$^{52}Cr^{65}$	12.46752	83.76	- 459
$^{50}Ti^{4}$	12.48620	05.45	-1859
$^{50}Cr^{4}$	12.48651	04.31	-1949
$^{50}V^{4}$	12.48679	00.24	-2038
$^{75}As^{6}$	12.48695	100.00	-2093
$^{40}Ca^{54}$	12.48831	96.97	-2710
$^{25}Mg^{2}$	12.49292	10.13	-----
$^{63}Cu^{5}$	12.58592	69.09	
$^{38}A^{3}$	12.65424	00.063	
$^{53}Cr^{65}$	12.70576	09.55	- 448
$^{51}V^{4}$	12.73599	99.76	-----
$^{17}O^{32}$	12.74935	00.037	+ 953
$^{23}Na^{53}$	12.77209	100.00	- 931
$^{64}Ni^{5}$	12.78559	01.08	-53E3
$^{64}Zn^{5}$	12.78583	48.89	-----
$^{41}K^{54}$	12.80057	06.88	+ 867
$^{29}Si^{43}$	12.87843	04.70	
$^{54}Cr^{65}$	12.94533	02.38	- 224
$^{54}Fe^{65}$	12.94551	05.82	- 225
$^{52}Cr^{4}$	12.98513	83.76	- 713
$^{65}Cu^{5}$	12.98556	30.91	- 731
$^{39}K^{3}$	12.98790	93.10	- 841
$^{26}Mg^{2}$	12.99130	11.17	-1078
^{13}C	13.00336	01.107	-----
^{12}CH	13.00782	98.878	+2916
$^{13}Li_2$	13.03112	13.74	+ 468
$^{55}Mn^{65}$	13.18513	100.00	- 265
$^{66}Zn^{5}$	13.18521	27.81	- 265
$^{53}Cr^{4}$	13.23516	09.55	-----
$^{40}A^{3}$	13.32080	99.60	-22E4
$^{40}Ca^{3}$	13.32086	96.97	-----
$^{40}K^{3}$	13.32133	00.012	+28E3
$^{30}Si^{43}$	13.32166	03.09	+17E3
$^{24}Mg^{53}$	13.32502	78.70	+3202
$^{67}Zn^{5}$	13.38543	04.11	
$^{56}Fe^{65}$	13.42439	91.66	
$^{54}Cr^{4}$	13.48472	02.38	-2230
$^{54}Fe^{4}$	13.48490	05.82	-2298
$^{27}Al^{2}$	13.49077	100.00	-----
$^{18}O^{32}$	13.49937	00.204	+1569

$^{68}Zn^{5}$	13.58497	18.57	
$^{41}K^{3}$	13.65394	06.88	-----
$^{57}Fe^{65}$	13.66450	02.19	+1293
$^{55}Mn^{4}$	13.73451	100.00	-----
$^{44}Ca^{54}$	13.73609	02.06	+8693
$^{31}P^{43}$	13.76612	100.00	+ 434
$^{69}Ga^{5}$	13.78514	60.4	+ 271
$^{58}Fe^{65}$	13.90400	00.33	
$^{56}Fe^{4}$	13.98374	91.66	- 724
$^{70}Ge^{5}$	13.98480	20.52	- 766
$^{70}Zn^{5}$	13.98508	00.62	- 778
$^{43}Ca^{3}$	13.98621	00.64	- 831
$^{28}Si^{2}$	13.98847	92.21	- 959
^{14}N	14.00307	99.634	-----
^{14}C	14.00324	LT.01	+82E3
^{13}CH	14.01113	01.107	+1726
$^{12}CH_2$	14.01565	98.863	+1113
$^{7}Li_2$	14.03200	85.71	+ 484
$^{32}S^{43}$	14.20981	95.0	- 593
$^{57}Fe^{4}$	14.23385	02.19	-----
$^{19}F^{32}$	14.24880	100.00	+ 952
$^{46}Ti^{54}$	14.36020	08.00	
$^{43}Ca^{3}$	14.31959	00.146	
$^{26}Mg^{53}$	14.43477	11.17	
$^{58}Fe^{4}$	14.48333	00.33	-2945
$^{58}Ni^{4}$	14.48384	69.18	-3256
$^{29}Si^{2}$	14.48825	04.70	-----
$^{44}Ca^{3}$	14.65183	02.06	-----
$^{47}Ti^{54}$	14.67242	07.29	+ 713
$^{59}Co^{4}$	14.73330	100.00	
$^{60}Ni^{4}$	14.98269	26.23	- 861
$^{48}Ti^{54}$	14.98373	73.98	- 916
$^{45}Sc^{3}$	14.98531	100.00	-1014
$^{30}Si^{2}$	14.98688	03.09	-1134
$^{27}Al^{53}$	14.98974	100.00	-1446
^{15}N	15.00011	00.366	-----
$^{12}CH_3$	15.02347	98.523	+ 642
^{14}NH	15.01090	99.509	+1390
$^{34}S^{43}$	15.09683	04.22	
$^{61}Ni^{4}$	15.23277	01.19	
$^{46}Ti^{3}$	15.31754	08.00	-43E3
$^{46}Ca^{3}$	15.31790	00.003	-----
$^{62}Ni^{4}$	15.48209	03.66	-3233
$^{31}P^{2}$	15.48688	100.00	-----
$^{35}Cl^{43}$	15.54171	75.529	-15E3
$^{28}Si^{53}$	15.54274	92.21	-----
$^{50}Ti^{54}$	15.60775	05.34	-----
$^{50}Cr^{54}$	15.60814	04.31	+40E3
$^{63}Cu^{4}$	15.73240	69.09	
$^{47}Ti^{3}$	15.65059	07.29	
$^{64}Ni^{4}$	15.98199	01.08	-1238
$^{64}Zn^{4}$	15.98229	48.89	-1267
$^{48}Ti^{3}$	15.98265	73.98	-1305
$^{48}Ca^{3}$	15.98413	00.185	-1491
$^{32}S^{2}$	15.98604	95.0	-1303
^{16}O	15.99491	99.759	-----
^{15}NH	16.00793	00.366	+1229
$^{14}NH_2$	16.01872	99.955	+ 671
$^{12}CH_4$	16.03130	98.344	+ 400
$^{29}Si^{53}$	16.09805	04.70	
$^{52}Cr^{54}$	16.23141	83.76	-30E3
$^{65}Cu^{4}$	16.23195	30.91	-----
$^{49}Ti^{3}$	16.31596	05.51	
$^{66}Zn^{4}$	16.48151	27.81	-3907
$^{33}S^{2}$	16.48573	00.76	-----
$^{53}Cr^{54}$	16.54395	09.55	
$^{50}Ti^{3}$	16.64826	05.34	-----
$^{50}Cr^{3}$	16.64868	04.31	+40E3
$^{50}V^{3}$	16.64905	00.24	+21E3
$^{30}Si^{53}$	16.65209	03.09	+4347
$^{67}Zn^{4}$	16.73178	04.11	
$^{54}Cr^{54}$	16.85590	02.38	-----
$^{54}Fe^{54}$	16.85613	05.82	+73E3
$^{68}Zn^{4}$	16.98122	18.57	- 949
$^{51}V^{3}$	16.98133	99.76	- 955
$^{34}S^{2}$	16.98393	04.22	-1118
^{17}O	16.99913	00.037	-----
^{16}OH	17.00274	99.747	+4709
$^{14}NH_3$	17.02655	99.593	+ 620
$^{55}Mn^{54}$	17.16814	100.000	
$^{31}P^{53}$	17.20765	100.000	
$^{23}Na^{32}$	17.24234	100.000	
$^{52}Cr^{3}$	17.31350	83.76	-----
$^{39}K^{43}$	17.31720	93.10	+4679

$^{56}Fe^{54}$	17.47967	91.66	-3680
$^{70}Zn^{4}$	17.48134	00.62	-5677
$^{35}Cl^{2}$	17.48442	75.529	-----
$^{53}Cr^{3}$	17.64688	09.55	
$^{40}Ca^{43}$	17.76115	96.97	-----
$^{32}S^{53}$	17.76226	95.0	+16E3
$^{57}Fe^{54}$	17.79231	02.19	+ 570
$^{54}Cr^{3}$	17.97962	02.38	- 921
$^{54}Fe^{3}$	17.97987	05.82	- 933
$^{36}S^{2}$	17.98354	00.014	-1152
$^{36}A^{2}$	17.98377	00.337	-1170
$^{24}Mg^{32}$	17.98878	78.70	-1734
^{18}O	17.99916	00.204	-----
$^{12}C^{2}_{3}$	18.00000	96.71	+21E3
H_2O	18.01056	99.747	+1579
^{6}LiC	18.01500	07.34	+1136
$^{9}Be_2$	18.02439	100.00	+ 713
$^{14}NH_4$	18.03437	99.584	+ 511
$^{58}Fe^{54}$	18.10416	00.33	
$^{41}K^{43}$	18.20526	06.88	
$^{55}Mn^{3}$	18.31269	100.00	
$^{37}Cl^{2}$	18.48295	24.471	-----
$^{37}C^{2}_{3}$	18.50168	3.25	+ 987
$^{56}Fe^{3}$	18.64498	91.66	
$^{25}Mg^{32}$	18.73938	10.13	
$^{34}S^{53}$	18.87103	04.22	
$^{57}Fe^{3}$	18.97847	02.19	- 953
$^{38}A^{2}$	18.98137	00.063	-1116
^{19}F	18.99840	100.00	-----
$^{38}C^{2}_{3}$	19.00336	00.036	+3830
^{18}OH	19.00698	00.204	+2214
H_2O	19.01477	00.037	+1161
^{19}LiC	19.01600	91.64	+1079
H_3O	19.01837	99.714	+ 951
$^{58}Fe^{3}$	19.31110	00.33	-28E3
$^{58}Ni^{3}$	19.31178	69.18	-----
$^{39}K^{2}$	19.48186	93.10	-----
$^{26}Mg^{32}$	19.48695	11.17	+3827
$^{44}Ca^{43}$	19.53577	02.06	+ 361
$^{60}Ni^{3}$	19.97692	26.23	-1288
$^{40}A^{2}$	19.98119	99.60	-1777
$^{40}Ca^{2}$	19.98129	96.97	-1793
$^{40}K^{2}$	19.98200	00.012	-1915
^{20}Ne	19.99244	90.92	-----
HF	20.00622	99.985	+1451
H_2O	20.01480	00.204	+ 894
$^{10}B_2$	20.02588	03.85	+ 598
$^{27}Al^{32}$	20.23616	100.00	
$^{61}Ni^{3}$	20.31036	01.19	
$^{46}Ti^{43}$	20.42339	08.00	
$^{41}K^{2}$	20.48092	06.88	
$^{62}Ni^{3}$	20.64278	03.66	
$^{47}Ti^{43}$	20.86745	07.29	
$^{63}Cu^{3}$	20.97653	69.09	-1212
$^{84}Sr^{4}$	20.97831	00.56	-1351
$^{42}Ca^{2}$	20.97931	00.64	-1444
$^{28}Si^{32}$	20.98270	92.21	-1383
^{21}Ne	20.99385	00.257	-----
^{9}BeC	21.01219	98.89	+1144
$^{21}B_2$	21.02225	31.52	+ 739
$^{85}Rb^{4}$	21.22801	72.15	
$^{64}Ni^{3}$	21.30932	01.08	-55E3
$^{64}Zn^{3}$	21.30971	48.89	-----
$^{48}Ti^{43}$	21.31020	73.98	+43E3
$^{86}Sr^{4}$	21.47734	09.86	-11E3
$^{43}Ca^{2}$	21.47939	00.146	-----
$^{65}Cu^{3}$	21.64259	30.91	-----
$^{39}K^{53}$	21.64650	93.10	+5535
$^{87}Sr^{4}$	21.72725	09.86	-27E4
$^{87}Rb^{4}$	21.72733	27.85	-----
$^{29}Si^{32}$	21.73237	04.70	+4311
$^{66}Zn^{3}$	21.97535	27.81	-9157
$^{88}Sr^{4}$	21.97650	82.56	-18E3
$^{44}Ca^{2}$	21.97775	02.06	-----
^{22}Ne	21.99138	08.82	+1612
^{6}LiO	22.00991	07.40	+ 683
^{10}BC	22.01294	19.39	+ 625
$^{11}B_2$	22.01861	64.63	+ 538
$^{50}Ti^{43}$	22.19768	05.34	- 773
$^{50}Cr^{43}$	22.19824	04.31	- 788
$^{40}Ca^{53}$	22.20143	96.97	- 339
$^{89}Y^{4}$	22.22643	100.00	-----
$^{67}Zn^{3}$	22.30905	04.11	

$^{90}Zr^{4}$	22.47608	51.48	-12E3
$^{45}Sc^{2}$	22.47796	100.00	-----
$^{30}Si^{32}$	22.48032	03.09	+9524
$^{68}Zn^{3}$	22.64162	18.57	
$^{91}Zr^{4}$	22.72633	11.22	-----
$^{41}K^{53}$	22.75657	06.88	+ 753
$^{69}Ga^{3}$	22.97524	60.4	-1581
$^{92}Zr^{4}$	22.97617	17.11	-1689
$^{46}Ti^{2}$	22.97632	08.00	-1708
$^{46}Ca^{2}$	22.97684	00.003	-1776
^{23}Na	22.98978	100.00	-----
^{23}BC	23.00931	79.72	+1177
^{7}LiO	23.01091	92.36	+1089
$^{52}Cr^{43}$	23.08467	83.76	
$^{93}Nb^{4}$	23.22642	100.00	-----
$^{31}P^{32}$	23.23032	100.00	+5955
$^{70}Ge^{3}$	23.30800	20.52	-----
$^{70}Zn^{3}$	23.30845	00.62	+52E3
$^{47}Ti^{2}$	23.47587	07.29	-----
$^{94}Zr^{4}$	23.47691	17.40	+23E3
$^{53}Cr^{43}$	23.52918	09.55	
$^{71}Ga^{3}$	23.64033	39.6	
$^{54}Cr^{43}$	23.97283	02.38	-1964
$^{54}Fe^{43}$	23.97316	05.82	-2019
$^{72}Ge^{3}$	23.97386	27.43	-2145
$^{48}Ti^{2}$	23.97397	73.98	-2167
$^{48}Ca^{2}$	23.97626	00.185	-2731
$^{96}Zr^{4}$	23.97733	02.80	-3111
$^{32}S^{32}$	23.97906	95.0	-4011
^{24}Mg	23.98504	78.70	-----
^{23}NaH	23.99760	99.985	+1910
$^{12}C_2$	24.00000	97.798	+1603
$^{73}Ge^{3}$	24.30778	07.76	
$^{55}Mn^{43}$	24.41691	100.00	-8690
$^{44}Ca^{53}$	24.41972	02.06	-----
$^{49}Ti^{2}$	24.47393	05.51	
$^{74}Ge^{3}$	24.64033	36.54	-----
$^{74}Se^{3}$	24.64085	00.87	+47E3
$^{56}Fe^{43}$	24.85997	91.66	
$^{50}Ti^{2}$	24.97239	05.34	-1858
$^{50}Cr^{2}$	24.97302	04.31	-1949
$^{50}V^{2}$	24.97358	00.24	-2038
$^{75}As^{3}$	24.97390	100.00	-2093
^{25}Mg	24.98584	10.13	-----
^{24}MgH	24.99760	78.69	+3559
$^{25}C_2$	25.00336	02.189	+1426
^{9}BeO	25.00711	99.759	+1175
$^{12}C_2H$	25.00782	97.786	+1137
$^{57}Fe^{43}$	25.30462	02.19	-10E3
$^{76}Se^{3}$	25.30643	09.02	-38E3
$^{76}Ge^{3}$	25.30710	07.76	-----
$^{51}V^{2}$	25.47199	99.76	-----
$^{34}S^{32}$	25.47590	04.22	+6515
$^{51}C^{2}_{4}$	25.50502	5.4E4	+ 771
$^{46}Ti^{53}$	25.52924	08.00	+ 445
$^{77}Se^{3}$	25.64000	07.58	
$^{58}Fe^{43}$	25.74814	00.33	
$^{52}Cr^{2}$	25.97026	83.76	-2107
$^{78}Se^{3}$	25.97246	23.52	-2565
$^{78}Kr^{3}$	25.97340	00.354	-2827
^{26}Mg	25.98259	11.17	-----
^{25}MgH	25.99366	10.13	+2347
^{12}CN	26.00307	98.54	+1269
$^{13}C_2$	26.00671	00.013	+1077
^{10}BO	26.00785	19.56	+1029
$^{12}C_2H_2$	26.01565	97.77	+ 786
$^{47}Ti^{53}$	26.08431	07.29	
$^{59}Co^{43}$	26.19252	100.00	- 769
$^{35}Cl^{32}$	26.22664	75.529	-----
$^{79}Br^{3}$	26.30613	50.537	
$^{53}Cr^{2}$	26.47032	09.55	
$^{60}Ni^{43}$	26.63590	26.23	-9123
$^{80}Se^{3}$	26.63882	49.82	-----
$^{80}Kr^{3}$	26.63886	02.27	+67E4
$^{48}Ti^{53}$	26.63775	73.98	-25E3
$^{54}Cr^{2}$	26.96944	02.38	-2230
$^{54}Fe^{2}$	26.96980	05.82	-2298
$^{81}Br^{3}$	26.97214	49.463	-2870
^{27}Al	26.98154	100.00	-----
^{26}MgH	26.99041	11.17	+3042
$^{12}C^{15}N$	27.00011	00.362	+1453
^{11}BO	27.00422	80.20	+1190
$^{13}C^{14}N$	27.00643	01.107	+1084
$^{12}C_2H_3$	27.02347	97.762	+ 643
$^{82}Kr^{3}$	27.30448	11.56	-26E3
$^{82}Se^{3}$	27.30554	09.19	-----
$^{55}Mn^{2}$	27.46903	100.00	
$^{83}Kr^{3}$	27.63802	11.55	
$^{50}Ti^{53}$	27.74710	05.34	-39E3
$^{50}Cr^{53}$	27.74781	04.31	-----
$^{56}Fe^{2}$	27.96747	91.66	-2957
$^{63}Cu^{43}$	27.96871	69.09	-3404
$^{84}Kr^{3}$	27.97050	56.90	-4351
$^{84}Sr^{3}$	27.97108	00.56	-4782
^{28}Si	27.97693	92.21	-----
^{27}AlH	27.98936	99.985	+2251
^{12}CO	27.99491	98.66	+1556
$^{14}N_2$	28.00615	99.269	+ 957
$^{12}C_2H_4$	28.03130	97.75	+ 524
$^{85}Rb^{3}$	28.30401	72.15	
$^{64}Zn^{43}$	28.41295	48.89	
$^{57}Fe^{2}$	28.46770	02.19	
$^{86}Sr^{3}$	28.63645	09.86	-----
$^{86}Kr^{3}$	28.63693	17.37	+60E3
$^{52}Cr^{53}$	28.35584	83.76	-----
$^{65}Cu^{43}$	28.35679	30.91	+30E3
$^{58}Fe^{2}$	28.96666	00.33	-2948
$^{58}Ni^{2}$	28.96768	69.18	-3289
$^{87}Sr^{3}$	28.96966	07.02	-4242
$^{87}Rb^{3}$	28.96977	27.85	-4312
^{29}Si	28.97649	04.70	-----
^{28}SiH	28.98475	92.20	+3508
^{13}CO	28.99827	01.104	+1330
$^{12}C^{17}O$	28.99910	00.037	+1282
^{12}CHO	29.00274	98.64	+1104
$^{29}N_2$	29.00318	00.73	+1086
$^{12}C_2H_5$	29.03912	97.74	+ 463
$^{39}K^{32}$	29.22278	93.10	
$^{88}Sr^{3}$	29.30200	82.56	
$^{53}Cr^{53}$	29.41147	09.55	
$^{59}Co^{2}$	29.46659	100.00	
$^{89}Y^{3}$	29.63524	100.00	
$^{60}Ni^{2}$	29.96538	26.23	-3577
$^{54}Cr^{53}$	29.96604	02.38	-3883
$^{54}Fe^{53}$	29.96645	05.82	-4100
$^{90}Zr^{3}$	29.96881	51.48	-5305
$^{40}Ca^{32}$	29.97194	96.97	-16E3
^{30}Si	29.97376	03.09	-----
^{29}SiH	29.98431	04.70	+2841
^{14}NO	29.99799	99.39	+1237
$^{12}C^{18}O$	29.99916	00.202	+1180
$^{60}C^{2}_{5}$	30.00000	94.57	+1142
$^{15}N_2$	30.00022	00.001	+1133
$^{12}CH_2O$	30.01056	99.63	+ 315
$^{6}LiC_2$	30.01500	07.26	+ 727
$^{12}C_2H_6$	30.04695	97.73	+ 410
$^{91}Zr^{3}$	30.30177	11.22	
$^{61}Ni^{2}$	30.46554	01.19	
$^{55}Mn^{53}$	30.52114	100.00	
$^{69}Ga^{43}$	30.63365	60.4	-25E3
$^{92}Zr^{3}$	30.63489	17.11	-----
$^{92}Mo^{3}$	30.63618	15.84	+24E3
$^{41}K^{32}$	30.72137	06.88	
$^{62}Ni^{2}$	30.96417	03.66	-3230
$^{93}Nb^{3}$	30.96855	100.00	-5945
^{31}P	30.97376	100.00	-----
^{30}SiH	30.98158	03.09	+3361
^{15}NO	30.99502	00.362	+1457
^{12}CF	30.99840	98.893	+1257
^{13}CO	31.00251	00.002	+1077
$^{62}C^{2}_{5}$	31.00336	00.119	+1046
$^{31}LiC_2$	31.01600	90.70	+ 733
$^{12}CH_3O$	31.01839	98.62	+ 694
$^{56}Fe^{53}$	31.07497	91.66	
$^{94}Mo^{3}$	31.30198	09.04	-55E3
$^{94}Zr^{3}$	31.30255	17.40	-----
$^{63}Cu^{2}$	31.46480	69.09	
$^{63}C^{2}_{5}$	31.50502	00.0013	
$^{57}Fe^{53}$	31.63078	02.19	-7849
$^{95}Mo^{3}$	31.63481	15.72	-----
$^{64}Ni^{2}$	31.96398	01.08	-3952
$^{64}Zn^{2}$	31.96457	48.89	-4263
$^{96}Mo^{3}$	31.96832	16.53	-8526
$^{96}Ru^{3}$	31.9696	05.51	-13E3
$^{96}Zr^{3}$	31.96977	02.80	-14E3
^{32}S	31.97207	95.0	-----
^{31}PH	31.98158	99.985	+3362
$^{16}O_2$	31.98983	99.52	+1800
$^{13}C^{19}F$	32.00176	01.11	+1077
$^{12}CH_4O$	32.02613	99.60	+ 591
$^{58}Fe^{53}$	32.18517	00.33	
$^{97}Mo^{3}$	32.30207	09.46	
$^{65}Cu^{2}$	32.46389	30.91	-----
$^{130}Ba^{4}$	32.47656	00.101	+2562
$^{98}Mo^{3}$	32.63533	23.78	-----
$^{98}Ru^{3}$	32.651/	01.87	+2083
$^{74}Ge^{43}$	32.85378	36.54	
$^{66}Zn^{2}$	32.96302	27.81	-3907
$^{44}Ca^{32}$	32.96662	02.06	-6812
$^{99}Ru^{3}$	32.96868	12.72	-12E3
^{33}S	32.97146	00.76	-----
$^{132}Ba^{4}$	32.97628	00.097	+6841
^{32}SH	32.97989	95.0	+3911
$^{33}O_2$	32.99405	00.075	+1460
$^{100}Ru^{3}$	33.302/	12.62	-20E4
$^{100}Mo^{3}$	33.30217	09.63	-----
$^{67}Zn^{2}$	33.46357	04.11	-----
$^{134}Ba^{4}$	33.47606	02.42	+2679
$^{101}Ru^{3}$	33.635/	17.07	
$^{135}Ba^{4}$	33.72639	06.59	
$^{68}Zn^{2}$	33.96243	18.57	-6256
^{34}S	33.96786	04.22	-----
$^{102}Ru^{3}$	33.96791	31.61	+68E4
$^{102}Pd^{3}$	33.96829	00.96	+79E3
$^{136}Ba^{4}$	33.97609	07.81	+4127
^{33}SH	33.97928	00.76	+2974
$^{34}O_2$	33.99408	00.407	+1295
$^{10}BC_2$	34.01294	19.18	+ 754
$^{137}Ba^{4}$	34.22639	11.32	
$^{103}Rh^{3}$	34.30152	100.00	
$^{69}Ga^{2}$	34.46286	60.4	-----
$^{46}Ti^{32}$	34.46447	08.00	+21E3
$^{138}Ba^{4}$	34.47622	71.66	+2580
$^{104}Pd^{3}$	34.63443	10.97	-----
$^{104}Ru^{3}$	34.63474	18.58	+11E4
$^{139}La^{4}$	34.72651	99.911	
$^{70}Ge^{2}$	34.96200	20.52	-5105
$^{70}Zn^{2}$	34.96267	00.62	-5658
$^{105}Pd^{3}$	34.96827	22.23	-60E3
^{35}Cl	34.96885	75.529	-----
^{34}SH	34.97568	04.22	+5120
$^{140}Ce^{4}$	34.97632	88.48	+4681
^{23}NaC	34.98978	98.89	+1669
^{19}FO	34.99331	99.76	+1430
$^{35}O_2$	34.99829	1.4E4	+1188
$^{35}BC_2$	35.00931	79.05	+ 864
$^{47}Ti^{32}$	35.21382	07.29	
$^{106}Pd^{3}$	35.30097	27.33	-----
$^{106}Cd^{3}$	35.30198	01.215	+35E3
$^{71}Ga^{2}$	35.46241	39.6	-----
$^{142}Ce^{4}$	35.47733	11.07	+2377
$^{107}Ag^{3}$	35.63495	51.35	
$^{72}Ge^{2}$	35.96080	27.43	-5718
$^{48}Ti^{32}$	35.96096	73.98	-5867
^{36}S	35.96709	00.014	-----
^{36}A	35.96755	00.337	+79E3
$^{108}Pd^{3}$	35.96782	26.71	+49E3
$^{1}H^{35}Cl$	35.97668	75.52	+3750
^{24}MgC	35.98504	77.83	+2008
$^{23}Na^{13}C$	35.99314	01.107	+1378
$^{36}C_3$	36.00000	96.71	+1093
$(NH_4)_2$	36.06874	-----	+ 354
$^{109}Ag^{3}$	36.30154	48.65	
$^{73}Ge^{2}$	36.46167	07.76	
$^{110}Cd^{3}$	36.63443	12.39	-----
$^{110}Pd^{3}$	36.63482	11.81	+94E3
$^{74}Ge^{2}$	36.96050	36.54	-6846
$^{74}Se^{2}$	36.96127	00.87	-7984
^{37}Cl	36.96590	24.471	-----
$^{111}Cd^{3}$	36.96809	12.75	+17E3
^{36}SH	36.97491	00.014	+5120
^{37}MgC	36.98584	11.00	+1858
$^{37}C_3$	37.00336	03.25	+ 987
$^{12}C_3H$	37.00782	96.70	+ 882
$^{112}Cd^{3}$	37.30102	24.07	-----
$^{112}Sn^{3}$	37.3017	00.96	+55E3
$^{50}Ti^{32}$	37.45859	05.34	-17E3
$^{50}Cr^{32}$	37.45954	04.31	-28E3
$^{75}As^{2}$	37.46086	100.00	-----
$^{113}In^{3}$	37.63477	04.28	-----
$^{113}Cd^{3}$	37.63482	12.26	+75E4
$^{85}Rb^{43}$	37.73868	72.15	
$^{76}Se^{2}$	37.95964	09.02	-12E3
$^{76}Ge^{2}$	37.96065	07.76	-18E3
^{38}A	37.96273	00.063	-----
$^{114}Cd^{3}$	37.96785	28.86	+7415
$^{114}Sn^{3}$	37.9680	00.66	+7204
$^{1}H^{37}Cl$	37.97373	24.467	+3450
^{38}MgC	37.98269	11.16	+1910
$^{25}Mg^{13}C$	37.98920	00.112	+1434
$^{19}F_2$	37.99680	100.00	+1114
$^{38}C_3$	38.00670	00.036	+ 863
$^{12}C_2{}^{14}N$	38.00307	97.43	+ 941
$^{12}C_3H_2$	38.01565	96.69	+ 717

$^{115}Sn^{3}$	38.30112	00.35	-48E4
$^{115}In^{3}$	38.30120	95.72	-----
$^{77}Se^{2}$	38.45999	07.58	
$^{116}Sn^{3}$	38.63406	14.30	-----
$^{116}Cd^{3}$	38.63500	07.58	+41E3
$^{52}Cr^{32}$	38.95538	83.76	-4678
$^{78}Se^{2}$	38.95870	23.52	-7777
$^{78}Kr^{2}$	38.96010	00.354	-11E3
^{39}K	38.96371	93.10	-----
$^{117}Sn^{3}$	38.96770	07.61	+9765
^{27}AlC	38.98154	98.89	+2190
^{23}NaO	38.98469	99.76	+1856
$^{26}Mg^{13}C$	38.98605	00.124	+1748
$^{12}C_2{}^{15}N$	39.00011	00.362	+1070
$^{7}LiO_2$	39.00581	92.13	+ 926
$^{13}C_3$	39.01005	01.4E4	+ 841
$^{12}C_3H_3$	39.02347	96.70	+ 652
$^{88}Sr^{43}$	39.06934	82.56	
$^{118}Sn^{3}$	39.30068	24.03	
$^{79}Br^{2}$	39.45920	50.537	
$^{89}Y^{43}$	39.51365	100.00	
$^{119}Sn^{3}$	39.63438	08.58	
$^{53}Cr^{32}$	39.70549	09.55	
$^{90}Zr^{43}$	39.95748	51.46	-7820
$^{80}Se^{2}$	39.95824	49.82	-9187
$^{80}Kr^{2}$	39.95830	02.27	-9315
^{40}A	39.96239	99.60	-20E4
^{40}Ca	39.96259	96.97	-----
^{40}K	39.96400	00.012	+28E3
$^{120}Sn^{3}$	39.96740	32.85	+8308
$^{120}Te^{3}$	39.96816	00.089	+7175
^{39}KH	39.97153	93.09	+4470
^{28}SiC	39.97693	91.19	+2993
^{24}MgO	39.97996	78.60	+2301
$^{27}Al^{13}C$	39.98489	98.89	+1791
$^{12}C_2O$	39.99491	97.56	+1236
$^{12}C_3H_4$	40.03130	95.60	+ 582
$^{121}Sb^{3}$	40.30124	57.25	
$^{54}Cr^{32}$	40.45415	02.38	-9965
$^{54}Fe^{32}$	40.45471	05.82	-12E3
$^{81}Br^{2}$	40.45821	49.463	-----
$^{122}Te^{3}$	40.63430	02.46	-21E4
$^{122}Sn^{3}$	40.63449	04.72	-----
$^{92}Zr^{43}$	40.84652	17.11	
$^{82}Kr^{2}$	40.95673	11.56	-8032
$^{82}Se^{2}$	40.95832	09.19	-12E3
^{41}K	40.96183	06.88	-----
$^{123}Sb^{3}$	40.96806	42.75	+6575
$^{123}Te^{3}$	40.9681	00.87	+6533
^{40}CaH	40.97041	96.96	+4774
^{40}KH	40.97182	00.012	+4100
^{41}SiC	40.97649	05.67	+2792
$^{23}Na^{18}O$	40.98894	00.204	+1508
$^{12}C_2{}^{17}O$	40.99910	00.037	+1099
$^{12}C_2HO$	41.00274	97.55	+1001
$^{9}BeO_2$	41.0020	99.52	+1020
$^{12}C_3H_5$	41.0391	96.66	+ 530
$^{55}Mn^{32}$	41.20354	100.00	
$^{124}Te^{3}$	41.30104	04.61	-58E3
$^{124}Sn^{3}$	41.30175	05.94	-----
$^{124}Xe^{3}$	41.30204	00.096	+14E4
$^{83}Kr^{2}$	41.45703	11.55	
$^{125}Te^{3}$	41.63487	06.99	
$^{94}Zr^{43}$	41.73673	17.40	
$^{56}Fe^{32}$	41.95120	91.66	-5647
$^{84}Kr^{2}$	41.95576	56.90	-15E3
$^{84}Sr^{2}$	41.95663	00.56	-20E3
^{42}Ca	41.95863	00.64	-----
$^{126}Te^{3}$	41.96796	18.71	+4497
$^{126}Xe^{3}$	41.96815	00.90	+4407
^{41}KH	41.96965	06.88	+3807
^{42}SiC	41.97649	03.11	+2766
^{26}MgO	41.97751	11.11	+2222
$^{24}Mg^{18}O$	41.98420	00.16	+1641
$^{12}C_2{}^{18}O$	41.99916	97.56	+1035
$^{84}C_7^{2}$	42.00000	92.48	+1014
$^{10}BO_2$	42.00274	19.52	+ 951
$^{12}C_2H_2O$	42.01056	97.54	+ 808
$^{12}C_3H_6$	42.04695	96.64	+ 475
$^{127}I^{3}$	42.30155	100.00	
$^{85}Rb^{2}$	42.45601	72.15	-----
$^{85}C_7^{2}$	42.50168	07.25	+ 930
$^{128}Xe^{3}$	42.63450	01.919	-63E3
$^{128}Te^{3}$	42.63518	31.79	-----
$^{57}Fe^{32}$	42.70155	02.19	
$^{86}Sr^{2}$	42.95468	09.86	-10E3
$^{86}Kr^{2}$	42.95540	17.37	-13E3
^{43}Ca	42.95878	00.146	-----

^{43}Ca	42.95878	00.146	-----
^{42}CaH	42.96645	00.64	+5601
$^{129}Xe^{3}$	42.96825	26.44	+4536
^{31}PC	42.97376	98.89	+2860
^{27}AlO	42.97645	99.76	+2431
$^{30}Si^{13}C$	42.97711	00.034	+2332
$^{25}Mg^{18}O$	42.98530	00.021	+1620
$^{12}C_2{}^{19}F$	42.9984	97.80	+1450
$^{11}BO_2$	42.99911	80.00	+1065
C_2H_3O	43.01839	97.53	+ 721
$^{12}C_3H_7$	43.05477	96.63	+ 448
$^{130}Xe^{3}$	43.30117	04.08	-48E3
$^{130}Ba^{3}$	43.30208	00.101	-----
$^{130}Te^{3}$	43.30232	34.48	+18E4
$^{58}Fe^{32}$	43.44999	00.33	-9635
$^{87}Sr^{2}$	43.45450	07.02	-----
$^{87}Rb^{2}$	43.45465	27.85	+29E4
$^{131}Xe^{3}$	43.63503	21.18	
$^{88}Sr^{2}$	43.95301	82.56	-18E3
^{44}Ca	43.95550	02.06	-----
^{43}CaH	43.96660	00.146	+3960
$^{132}Ba^{3}$	43.96837	00.097	+3415
$^{132}Xe^{3}$	43.96805	26.89	+3502
^{28}SiO	43.97184	91.99	+2690
^{32}SC	43.97207	94.0	+2653
$^{31}P^{13}C$	43.97711	01.107	+2026
$^{26}Mg^{18}O$	43.98175	00.023	+1674
CO_2	43.98983	97.8	+1280
C_2H_4O	44.02621	97.51	+ 622
C_3H_8	44.06260	96.62	+ 410
$^{59}Co^{32}$	44.19989	100.00	
$^{133}Cs^{3}$	44.30171	100.00	
$^{89}Y^{2}$	44.45286	100.00	
$^{134}Ba^{3}$	44.63475	02.42	-----
$^{134}Xe^{3}$	44.63514	10.44	+11E4
$^{60}Ni^{32}$	44.94808	26.23	-5734
$^{90}Zr^{2}$	44.95217	51.46	-12E3
^{45}Sc	44.95592	100.00	-----
^{44}CaH	44.96332	02.06	+6075
$^{135}Ba_3$	44.96852	06.59	+3568
^{29}SiO	44.97141	04.69	+2902
^{45}SC	44.97542	01.80	+2305
^{27}AlO	44.98070	00.204	+1814
$^{45}CO_2$	44.99318	01.176	+1207
$^{12}C_2H_5O$	45.03404	97.50	+ 575
$^{136}Ba^{3}$	45.30146	07.81	-----
$^{136}Ce^{3}$	45.30236	00.193	+50E3
$^{136}Xe^{3}$	45.30240	08.87	+48E3
$^{91}Zr^{2}$	45.45266	11.22	
$^{137}Ba^{3}$	45.63519	11.32	
$^{92}Zr^{2}$	45.95234	17.11	-16E4
^{46}Ti	45.95263	08.00	-----
^{46}Ca	45.95369	03.3E3	+43E3
$^{92}Mo^{2}$	45.95428	15.84	+28E3
^{45}ScH	45.96374	99.985	+4136
^{34}SC	45.96786	04.17	+3020
$^{138}Ba^{3}$	45.96829	71.66	+2934
^{30}SiO	45.96867	03.08	+2865
$^{138}Ce^{3}$	45.96868	00.25	+2863
$^{138}La^{3}$	45.96891	00.089	+2827
$^{28}Si^{18}O$	45.97609	00.188	+1958
$^{23}Na_2$	45.97956	100.00	+1706
$^{14}NO_2$	45.99290	99.15	+1141
C_2H_6O	46.04186	97.49	+ 515
$^{139}La^{3}$	46.30201	99.911	
$^{93}Nb^{2}$	46.45283	100.000	
$^{140}Ce^{3}$	46.63509	88.48	
^{47}Ti	46.95176	07.29	-----
$^{94}Zr^{2}$	46.95382	17.40	+23E3
$^{94}Mo^{2}$	46.95297	09.04	+39E3
^{46}TiH	46.96045	08.00	+5403
^{31}PO	46.96872	99.76	+2768
^{35}ClC	46.96885	74.69	+2747
$^{141}Pr^{3}$	46.96916	100.00	+2698
$^{29}Si^{18}O$	46.97565	00.01	+1961
$^{23}NaC_2$	46.98978	97.80	+1234
$^{15}NO_2$	46.98991	00.36	+1231
$^{63}Cu^{32}$	47.19720	69.09	
$^{142}Nd^{3}$	47.30249	27.11	-78E3
$^{142}Ce^{3}$	47.30310	11.07	-----
$^{95}Mo^{2}$	47.45222	15.72	
$^{143}Nd^{3}$	47.63653	12.17	
$^{64}Zn^{32}$	47.94686	48.89	-44E3
^{48}Ti	47.94795	73.98	-----
$^{96}Mo^{2}$	47.95248	16.53	+11E3
^{48}Ca	47.95253	00.185	+10E3
$^{96}Ru^{2}$	47.9544	05.51	+7434
$^{96}Zr^{2}$	47.95465	02.80	+7156
^{47}TiH	47.95958	07.29	+4123
^{32}SO	47.96699	94.8	+2518

^{36}SC	47.96709	00.013	+2505
$^{144}Nd^{3}$	47.96993	23.85	+2181
$^{24}Mg_2$	47.97008	61.94	+2167
$^{144}Sm^{3}$	47.97055	03.09	+2122
$^{35}Cl^{13}C$	47.97220	00.84	+1977
$^{30}Si^{18}O$	47.97292	00.006	+1914
$^{16}O_3$	47.98473	99.28	+1304
$^{24}MgC_2$	47.98504	76.97	+1294
$^{12}C_4$	48.00000	95.63	+ 921
$^{145}Nd^{3}$	48.30402	08.30	
$^{97}Mo^{2}$	48.45311	09.46	
$^{97}C_8^{2}$	48.50168	07.25	
$^{146}Nd^{3}$	48.63756	17.22	-----
$^{65}Cu^{32}$	48.69584	30.91	+ 834
^{49}Ti	48.94787	05.51	-----
$^{98}Mo^{2}$	48.95299	23.78	+9560
^{48}TiH	48.95577	73.97	+6196
^{37}ClC	48.96590	24.20	+2715
^{49}SO	48.96640	00.80	+2641
$^{49}Mg_2$	48.97088	15.95	+2127
$^{147}Sm^{3}$	48.97150	14.97	+2071
$^{98}Ru^{2}$	48.977	01.87	+1680
$^{49}MgC_2$	48.98584	11.63	+1290
$^{49}O_3$	48.98892	00.11	+1192
$^{49}C_4$	49.00336	04.29	+ 882
$^{12}C_4H$	49.00782	95.62	+ 816
$^{148}Sm^{3}$	49.30481	11.24	-----
$^{148}Nd^{3}$	49.30549	05.73	+73E3
$^{99}Ru^{2}$	49.45303	12.72	
$^{149}Sm^{3}$	49.63893	13.83	
^{50}Ti	49.94479	05.34	-----
^{50}Cr	49.94605	04.31	+40E3
^{50}V	49.94716	00.24	+21E3
$^{100}Ru^{2}$	49.953	12.62	+6083
$^{100}Mo^{2}$	49.95326	09.63	+5897
^{49}TiH	49.95569	05.51	+4582
^{34}SO	49.96278	04.21	+2776
$^{50}Mg_2$	49.96763	18.61	+2187
^{37}ClC	49.96926	00.27	+2041
$^{23}NaAl$	49.97132	100.00	+1883
$^{150}Sm^{3}$	49.97230	07.44	+1815
$^{150}Nd^{3}$	49.97361	05.62	+1733
$^{50}MgC_2$	49.98259	11.16	+1321
$^{50}O_3$	49.98898	00.61	+1130
$^{12}CF_2$	49.99680	98.89	+ 960
$^{50}C_4$	50.00670	00.072	+ 806
$^{12}C_4H_2$	50.01564	95.61	+ 705
$^{151}Eu^{3}$	50.30651	47.82	
$^{101}Ru^{2}$	50.453	17.07	
$^{152}Sm^{3}$	50.63979	26.72	
$^{152}Gd^{3}$	50.63981	00.20	
^{51}V	50.94398	99.76	-----
$^{102}Ru^{2}$	50.95187	31.61	+6457
$^{102}Pd^{2}$	50.95243	00.96	+6029
^{50}TiH	50.95261	05.34	+5903
^{50}CrH	50.95388	04.31	+5151
^{39}KC	50.96371	92.07	+2582
^{35}ClO	50.96376	75.35	+2576
$^{24}MgAl$	50.96653	78.70	+2254
$^{28}SiNa$	50.96671	92.21	+2241
$^{51}Mg_2$	50.96843	02.26	+2034
$^{153}Eu^{3}$	50.9735	52.18	+1726
$^{27}AlC_2$	50.98154	97.80	+1358
$^{19}FO_2$	50.98822	99.52	+1152
$^{13}CF_2$	51.00016	01.11	+ 907
$^{51}C_4$	51.01005	05.4E4	+ 771
C_4H_3	51.02346	95.61	+ 641
$^{154}Gd^{3}$	51.30698	02.15	-16E4
$^{154}Sm^{3}$	51.30731	22.71	-----
$^{103}Rh^{2}$	51.45228	100.00	-----
$^{206}Pb^{4}$	51.49361	23.6	+1245
$^{155}Gd^{3}$	51.6409	14.73	-----
$^{69}Ga^{32}$	51.69428	60.4	+ 967
$^{207}Pb^{4}$	51.74397	22.6	
^{52}Cr	51.94051	83.76	-----
$^{104}Pd^{2}$	51.95164	10.97	+4667
^{51}VH	51.95180	99.985	+4601
$^{104}Ru^{2}$	51.95211	18.58	+4478
$^{28}SiMg$	51.96197	72.57	+2420
^{36}SO	51.96200	00.014	+2417
^{40}CaC	51.96259	95.90	+2352
$^{26}Mg_2$	51.96518	01.25	+2105
$^{25}MgAl$	51.96738	10.13	+1933
^{52}KC	51.96706	01.04	+1956
$^{156}Dy^{3}$	51.971/	00.052	+1704
$^{156}Gd^{3}$	51.97409	20.47	+1547
$^{28}SiC_2$	51.97693	90.18	+1427
$^{208}Pb^{4}$	51.99416	52.3	+ 968
$^{12}C_3O$	51.99492	96.43	+ 955
$^{12}C_4H_4$	52.03128	95.60	+ 572

$^{157}\mathrm{Gd}^{3}$	52.3080	15.68	
$^{105}\mathrm{Pd}^{2}$	52.45241	22.23	
$^{158}\mathrm{Dy}^{3}$	52.64134	00.09	
$^{158}\mathrm{Gd}^{3}$	52.6415	24.87	
$^{53}\mathrm{Cr}$	52.94065	09.55	-----
$^{52}\mathrm{CrH}$	52.94833	83.75	+6893
$^{106}\mathrm{Pd}^{2}$	52.95146	27.33	+4897
$^{106}\mathrm{Cd}^{2}$	52.95297	01.215	+4297
$^{37}\mathrm{ClO}$	52.96081	24.41	+2626
$^{41}\mathrm{KC}$	52.96183	06.80	+2500
$^{26}\mathrm{MgAl}$	52.96413	11.17	+2255
$^{40}\mathrm{Ca}^{13}\mathrm{C}$	52.96594	01.07	+2093
$^{159}\mathrm{Tb}^{3}$	52.97496	100.00	+1543
$^{53}\mathrm{SiC_2}$	52.97649	06.61	+1477
$\mathrm{C_4H_5}$	53.03910	95.05	+ 538
$^{160}\mathrm{Dy}^{3}$	53.3080	02.294	-50E3
$^{160}\mathrm{Gd}^{3}$	53.30907	21.90	-----
$^{107}\mathrm{Ag}^{2}$	53.45242	51.35	
$^{161}\mathrm{Dy}^{3}$	53.6419	18.88	
$^{54}\mathrm{Cr}$	53.93887	02.38	-73E3
$^{54}\mathrm{Fe}$	53.93961	05.82	-----
$^{53}\mathrm{CrH}$	53.94847	09.55	+6088
$^{108}\mathrm{Pd}^{2}$	53.95174	26.71	+4445
$^{108}\mathrm{Cd}^{2}$	53.95204	00.875	+4338
$^{42}\mathrm{CaC}$	53.95863	00.63	+2835
$^{27}\mathrm{Al_2}$	53.96306	100.00	+2300
$^{41}\mathrm{K}^{13}\mathrm{C}$	53.96518	00.076	+2109
$^{54}\mathrm{SiC_2}$	53.97376	03.12	+1577
$^{162}\mathrm{Dy}^{3}$	53.9752	25.53	+1515
$^{162}\mathrm{Er}^{3}$	53.97624	00.136	+1472
$^{12}\mathrm{C}_9^{2}$	54.00000	90.44	+ 893
$\mathrm{C_4H_6}$	54.04692	95.57	+ 499
$^{109}\mathrm{Ag}^{2}$	54.45231	48.65	-----
$^{109}\mathrm{C}_9^{2}$	54.50168	09.12	+1103
$^{164}\mathrm{Dy}^{3}$	54.64283	28.18	-----
$^{164}\mathrm{Er}^{3}$	54.64327	01.56	+12E4
$^{74}\mathrm{Ge}^{32}$	54.69251	36.54	+1100
$^{55}\mathrm{Mn}$	54.93805	100.00	-----
$^{54}\mathrm{CrH}$	54.94699	02.38	+6359
$^{54}\mathrm{FeH}$	54.94743	05.82	+5857
$^{110}\mathrm{Cd}^{2}$	54.95165	12.39	+4040
$^{28}\mathrm{SiAl}$	54.95847	92.88	+2990
$^{110}\mathrm{Pd}^{2}$	54.95224	11.81	+3872
$^{39}\mathrm{KO}$	54.95862	92.88	+2671
$^{165}\mathrm{Ho}^{3}$	54.95862	100.00	+2671
$^{55}\mathrm{CaC}$	54.95878	00.151	+2650
$^{31}\mathrm{PC_2}$	54.97376	97.80	+1537
$^{23}\mathrm{NaO_2}$	54.97960	99.52	+1322
$^{110}\mathrm{C}_9^{2}$	55.00335	00.41	+ 841
$^{12}\mathrm{C_4H_7}$	55.05474	95.56	+ 471
$^{166}\mathrm{Er}^{3}$	55.3096	33.41	
$^{111}\mathrm{Cd}^{2}$	55.45214	12.75	
$^{167}\mathrm{Er}^{3}$	55.6435	22.94	
$^{56}\mathrm{Fe}$	55.93494	91.66	-----
$^{55}\mathrm{MnH}$	55.94587	99.985	+5118
$^{112}\mathrm{Cd}^{2}$	55.95153	24.07	+3372
$^{112}\mathrm{Sn}^{2}$	55.9526	00.96	+3167
$^{28}\mathrm{Si_2}$	55.95386	85.03	+2956
$^{44}\mathrm{CaC}$	55.95550	02.04	+2788
$^{40}\mathrm{CaO}$	55.95750	96.51	+2479
$^{29}\mathrm{SiAl}$	55.95803	04.70	+2422
$^{40}\mathrm{KO}$	55.95891	00.018	+2334
$^{32}\mathrm{SC_2}$	55.97207	92.91	+1506
$^{24}\mathrm{MgO_2}$	55.97485	78.32	+1400
$^{168}\mathrm{Er}^{3}$	55.9769	27.07	+1333
$^{168}\mathrm{Yb}^{3}$	55.97797	00.135	+1300
$\mathrm{C_4H_8}$	56.06256	95.55	+ 438
$^{169}\mathrm{Tm}^{3}$	56.31145	100.00	
$^{113}\mathrm{In}^{2}$	56.45215	04.28	-71E4
$^{113}\mathrm{Cd}^{2}$	56.45223	12.26	-----
$^{170}\mathrm{Yb}^{3}$	56.645/	03.03	-28E4
$^{170}\mathrm{Er}^{3}$	56.6452	14.88	-----
$^{57}\mathrm{Fe}$	56.93541	02.19	-----
$^{56}\mathrm{FeH}$	56.94276	91.65	+7746
$^{114}\mathrm{Cd}^{2}$	56.95178	28.86	+3478
$^{114}\mathrm{Sn}^{2}$	56.9520	00.66	+3432
$^{57}\mathrm{Si_2}$	56.95342	08.66	+3161
$^{30}\mathrm{SiAl}$	56.95530	03.09	+2863
$^{45}\mathrm{ScC}$	56.95592	98.89	+2776
$^{41}\mathrm{KO}$	56.95674	06.86	+2669
$^{44}\mathrm{Ca}^{13}\mathrm{C}$	56.95835	00.023	+2482
$^{39}\mathrm{K}^{18}\mathrm{O}$	56.96287	00.19	+2071
$^{57}\mathrm{SC_2}$	56.97542	02.82	+1423
$^{25}\mathrm{MgO_2}$	56.97566	10.08	+1415
$^{171}\mathrm{Yb}^{3}$	56.979/	14.31	+1306
$\mathrm{C_4H_9}$	57.07038	95.54	+ 422
$^{172}\mathrm{Yb}^{3}$	57.3084/	21.82	
$^{115}\mathrm{Sn}^{2}$	57.45168	00.35	-44E4
$^{115}\mathrm{In}^{2}$	57.45181	95.72	-----
$^{173}\mathrm{Yb}^{3}$	57.646/	16.13	
$^{58}\mathrm{Fe}$	57.93331	00.33	-28E3
$^{58}\mathrm{Ni}$	57.93535	69.18	-----
$^{57}\mathrm{FeH}$	57.94323	02.19	+7352
$^{58}\mathrm{Si_2}$	57.95069	05.92	+3777
$^{116}\mathrm{Sn}^{2}$	57.95110	14.30	+3678
$^{116}\mathrm{Cd}^{2}$	57.95250	07.58	+3378
$^{46}\mathrm{CaC}$	57.95369	03.3E3	+3159
$^{46}\mathrm{TiC}$	57.95263	07.91	+3353
$^{42}\mathrm{CaO}$	57.95340	00.64	+3208
$^{40}\mathrm{Ca}^{18}\mathrm{O}$	57.96202	00.20	+2172
$^{34}\mathrm{SC_2}$	57.96786	04.13	+1782
$^{26}\mathrm{MgO_2}$	57.97241	11.12	+1564
$^{174}\mathrm{Yb}^{3}$	57.9752/	31.84	+1454
$^{23}\mathrm{Na_2C}$	57.97976	98.89	+1305
$^{174}\mathrm{Hf}^{3}$	57.980/	00.18	+1298
$^{175}\mathrm{Lu}^{3}$	58.314/	97.41	
$^{117}\mathrm{Sn}^{2}$	58.45155	07.61	
$^{176}\mathrm{Hf}^{3}$	58.6469	05.20	-88E3
$^{176}\mathrm{Lu}^{3}$	58.6473	02.59	-22E4
$^{176}\mathrm{Yb}^{3}$	58.64757	12.73	-----
$^{59}\mathrm{Co}$	58.93318	100.00	-----
$^{58}\mathrm{FeH}$	58.94113	00.33	+7413
$^{58}\mathrm{NiH}$	58.94317	69.17	+5899
$^{59}\mathrm{Si_2}$	58.95025	00.30	+3452
$^{28}\mathrm{SiP}$	58.95069	92.21	+3366
$^{118}\mathrm{Sn}^{2}$	58.95103	24.03	+3302
$^{59}\mathrm{TiC}$	58.95176	07.29	+3172
$^{43}\mathrm{CaO}$	58.95369	00.146	+2873
$^{41}\mathrm{K}^{18}\mathrm{O}$	58.96099	00.014	+2118
$^{35}\mathrm{ClC_2}$	58.96885	73.87	+1652
$^{27}\mathrm{AlO_2}$	58.97136	99.52	+1544
$^{177}\mathrm{Hf}^{3}$	58.9808	18.50	+1238
$^{23}\mathrm{NaC_3}$	58.98978	96.72	+1041
$^{178}\mathrm{Hf}^{3}$	59.3143	27.14	
$^{119}\mathrm{Sn}^{2}$	59.45158	08.58	
$^{179}\mathrm{Hf}^{3}$	59.6484	13.75	
$^{60}\mathrm{Ni}$	59.93077	26.23	-----
$^{59}\mathrm{CoH}$	59.94100	99.985	+5858
$^{30}\mathrm{Si_2}$	59.94752	00.10	+3578
$^{60}\mathrm{TiC}$	59.94795	73.24	+3488
$^{28}\mathrm{SiS}$	59.94900	87.60	+3287
$^{44}\mathrm{CaO}$	59.95041	02.06	+3051
$^{135}\mathrm{Ba}^{43}$	59.95082	06.59	+2889
$^{120}\mathrm{Sn}^{2}$	59.95110	32.58	+2948
$^{120}\mathrm{Te}$	59.95225	00.089	+2790
$^{48}\mathrm{CaC}$	59.95253	00.183	+2754
$^{28}\mathrm{SiO_2}$	59.96676	91.77	+1665
$^{36}\mathrm{SC_2}$	59.96709	00.013	+1650
$^{24}\mathrm{Mg_2C}$	59.97008	60.57	+1525
$^{180}\mathrm{W}^{3}$	59.9815	00.135	+1181
$^{180}\mathrm{Ta}^{3}$	59.982/	00.012	+1170
$^{180}\mathrm{Hf}^{3}$	59.9820	35.24	+1170
$^{12}\mathrm{CO_3}$	59.98473	98.18	+1111
$^{24}\mathrm{MgC_3}$	59.98504	76.12	+1105
$^{60}\mathrm{C_5}$	60.00000	94.57	+ 866
$^{181}\mathrm{Ta}^{3}$	60.3153	99.988	
$^{136}\mathrm{Ba}^{43}$	60.40194	07.81	
$^{121}\mathrm{Sb}^{2}$	60.45186	57.25	
$^{182}\mathrm{W}^{3}$	60.6487	26.41	
$^{137}\mathrm{Ba}^{43}$	60.84692	11.32	
$^{61}\mathrm{Ni}$	60.93109	01.19	-----
$^{60}\mathrm{NiH}$	60.93859	26.23	+8124
$^{61}\mathrm{TiC}$	60.94787	06.27	+3631
$^{45}\mathrm{ScO}$	60.95083	99.76	+3087
$^{122}\mathrm{Te}^{2}$	60.95145	04.72	+2993
$^{122}\mathrm{Sn}^{2}$	60.95173	04.72	+2952
$^{37}\mathrm{ClC_2}$	60.96590	23.93	+1750
$^{29}\mathrm{SiO_2}$	60.96632	04.68	+1730
$^{61}\mathrm{Mg_2C}$	60.97088	16.29	+1531
$^{183}\mathrm{W}^{3}$	60.9827	14.40	+1180
$^{13}\mathrm{CO_3}$	60.98809	01.10	+1069
$^{61}\mathrm{MgC_3}$	60.98584	12.48	+1114
$^{61}\mathrm{C_5}$	61.00336	05.30	+ 843
$^{12}\mathrm{C_5H}$	61.00782	94.56	+ 794
$^{138}\mathrm{Ba}^{43}$	61.29106	71.66	-2429
$^{184}\mathrm{Os}^{3}$	61.315/	00.018	-47E3
$^{184}\mathrm{W}^{3}$	61.3163	30.64	-----
$^{123}\mathrm{Sb}^{2}$	61.45209	42.75	-----
$^{123}\mathrm{Te}^{2}$	61.4522	00.87	+56E4
$^{185}\mathrm{Re}^{3}$	61.649/	37.07	+ 312
$^{139}\mathrm{La}^{43}$	61.73601	99.911	
$^{62}\mathrm{Ni}$	61.92834	03.66	-----
$^{61}\mathrm{NiH}$	61.93891	01.19	+5859
$^{50}\mathrm{CrC}$	61.94065	04.26	+5031
$^{62}\mathrm{TiC}$	61.94479	05.34	+3765
$^{50}\mathrm{VC}$	61.94716	00.24	+3291
$^{31}\mathrm{P_2}$	61.94753	100.00	+3227
$^{46}\mathrm{CaO}$	61.94754	3.3E3	+3225
$^{46}\mathrm{TiO}$	61.94854	07.27	+3066
$^{124}\mathrm{Te}^{2}$	61.95156	04.61	+2667
$^{124}\mathrm{Sn}^{2}$	61.95262	05.94	+2551
$^{124}\mathrm{Xe}^{2}$	61.95306	00.096	+2505
$^{30}\mathrm{SiO_2}$	61.96359	03.07	+1757
$^{62}\mathrm{Mg_2C}$	61.96763	18.19	+1576
$^{23}\mathrm{Na_2O}$	61.97447	99.76	+1343
$^{62}\mathrm{MgC_3}$	61.98259	11.25	+1141
$^{186}\mathrm{W}^{3}$	61.9836	28.41	+1121
$^{186}\mathrm{Os}^{3}$	61.984	01.59	+1113
$^{14}\mathrm{NO_3}$	61.98780	98.91	+1042
$^{62}\mathrm{C_5}$	62.00670	00.119	+ 790
$^{12}\mathrm{C_5H_2}$	62.01564	94.55	+ 709
$^{140}\mathrm{Ce}^{43}$	62.18012	88.48	
$^{187}\mathrm{Re}^{3}$	62.318/	62.93	-----
$^{187}\mathrm{Os}^{3}$	62.319/	01.64	+62E3
$^{125}\mathrm{Te}^{2}$	62.45231	06.99	
$^{188}\mathrm{Os}^{3}$	62.6523	13.3	
$^{63}\mathrm{Cu}$	62.92959	69.09	-----
$^{62}\mathrm{NiH}$	62.93616	03.66	+9578
$^{51}\mathrm{VC}$	62.94398	98.66	+4373
$^{47}\mathrm{TiO}$	62.94667	07.26	+3684
$^{50}\mathrm{Ti}^{13}\mathrm{C}$	62.94814	00.059	+3392
$^{50}\mathrm{Cr}^{13}\mathrm{C}$	62.94940	00.048	+3177
$^{126}\mathrm{Te}^{2}$	62.95194	18.71	+2816
$^{126}\mathrm{Xe}^{2}$	62.95223	00.09	+2780
$^{31}\mathrm{PO_2}$	62.96358	99.52	+1850
$^{39}\mathrm{KC_2}$	62.96371	91.05	+1844
$^{27}\mathrm{AlC_3}$	62.98154	96.72	+1212
$^{189}\mathrm{Os}^{3}$	62.9862/	16.1	+1112
$^{63}\mathrm{C_5}$	63.01008	01.3E3	+ 782
$\mathrm{C_5H_3}$	63.02346	94.55	+ 670
$^{190}\mathrm{Os}^{3}$	63.3183	26.4	-----
$^{190}\mathrm{Pt}^{3}$	63.321/	00.013	+24E3
$^{127}\mathrm{I}^{2}$	63.45233	100.00	
$^{191}\mathrm{Ir}^{3}$	63.6545	37.3	-2157
$^{85}\mathrm{Rb}^{32}$	63.68402	72.15	-----
$^{64}\mathrm{Ni}$	63.92796	01.08	-54E3
$^{64}\mathrm{Zn}$	63.92914	48.89	-----
$^{63}\mathrm{CuH}$	63.93741	69.08	+7730
$^{52}\mathrm{CrC}$	63.94051	82.83	+5623
$^{48}\mathrm{TiO}$	63.94286	73.76	+4660
$^{32}\mathrm{S_2}$	63.94414	90.25	+4262
$^{48}\mathrm{CaO}$	63.94744	00.185	+3493
$^{24}\mathrm{Mg}^{40}\mathrm{Ca}$	63.94790	76.32	+3408
$^{128}\mathrm{Xe}^{2}$	63.95176	01.919	+2826
$^{46}\mathrm{Ti}^{18}\mathrm{O}$	63.95179	00.016	+2821
$^{128}\mathrm{Te}^{2}$	63.95278	31.79	+2704
$^{32}\mathrm{SO_2}$	63.96190	94.54	+1951
$^{40}\mathrm{CaC_2}$	63.96259	94.83	+1911
$^{40}\mathrm{KC_2}$	63.96706	02.05	+1686
$^{24}\mathrm{Mg_2O}$	63.96499	61.79	+1783
$^{28}\mathrm{SiC_3}$	63.97693	89.18	+1339
$^{192}\mathrm{Os}^{3}$	63.9874	41.0	+1097
$^{192}\mathrm{Pt}^{3}$	63.9883	00.78	+1081
$^{12}\mathrm{C_4O}$	63.99491	95.41	+ 972
$\mathrm{C_5H_4}$	64.03128	94.52	+ 626
$^{193}\mathrm{Ir}^{3}$	64.3222	62.7	
$^{129}\mathrm{Xe}^{2}$	64.45237	26.44	
$^{194}\mathrm{Pt}^{3}$	64.6544/	32.9	
$^{65}\mathrm{Cu}$	64.92778	30.91	-----
$^{64}\mathrm{NiH}$	64.93578	01.08	+8116
$^{64}\mathrm{ZnH}$	64.93696	48.88	+7072
$^{53}\mathrm{CrC}$	64.94065	09.44	+5045
$^{49}\mathrm{TiO}$	64.94278	05.50	+4329
$^{65}\mathrm{S_2}$	64.94354	01.44	+4120
$^{52}\mathrm{Cr}^{13}\mathrm{C}$	64.94386	00.927	+4038
$^{47}\mathrm{Ti}^{18}\mathrm{O}$	64.95092	00.015	+2808
$^{130}\mathrm{Xe}^{2}$	64.95175	04.08	+2709
$^{130}\mathrm{Ba}^{2}$	64.95312	00.101	+2562
$^{130}\mathrm{Te}^{2}$	64.95348	34.48	+2526
$^{41}\mathrm{KC_2}$	64.96183	06.73	+1907
$^{49}\mathrm{Mg_2O}$	64.96597	15.91	+1700
$^{65}\mathrm{SiC_3}$	64.97649	07.55	+1333
$^{195}\mathrm{Pt}^{3}$	64.9887	33.8	+1066
$\mathrm{C_5H_5}$	65.03910	94.51	+ 583
$^{196}\mathrm{Hg}^{3}$	65.32194	00.146	-13E4
$^{196}\mathrm{Pt}^{3}$	65.3224	25.3	-----
$^{131}\mathrm{Xe}^{2}$	65.45354	21.18	
$^{197}\mathrm{Au}^{3}$	65.6557	100.00	
$^{66}\mathrm{Zn}$	65.92605	27.81	-----
$^{88}\mathrm{Sr}^{32}$	65.92951	82.56	+19E3
$^{65}\mathrm{CuH}$	65.93560	30.91	+6903
$^{54}\mathrm{CrC}$	65.93887	02.35	+5142
$^{54}\mathrm{FeC}$	65.93961	05.76	+4862
$^{50}\mathrm{TiO}$	65.93970	05.32	+4829
$^{66}\mathrm{S_2}$	65.93993	08.02	+4750
$^{50}\mathrm{CrO}$	65.94096	04.30	+4422

^{50}VO	65.94207	00.24	+4115
^{33}S$_2$	65.94293	00.006	+3906
^{53}Cr^{13}C	65.94401	00.106	+3673
^{39}KAl	65.94525	93.10	+3434
^{48}Ti^{18}O	65.94711	00.151	+3132
^{132}Xe^2	65.95208	26.89	+2533
^{132}Ba^2	65.95256	00.097	+2487
^{34}SO$_2$	65.95769	04.20	+2024
^{50}Mg$_2$O	65.96254	13.53	+1809
^{25}Mg$_2$O	65.96659	01.03	+1626
^{27}Al$_2$C	65.96308	98.90	+1780
^{66}SiC$_3$	65.97376	03.14	+1381
^{198}Pt^3	65.9738	07.21	+1381
^{198}Hg^3	65.98392	10.02	+1049
^{12}C$^{2}_{11}$	66.00000	88.45	+ 891
C$_5$H$_6$	66.04692	94.50	+ 545
^{199}Hg^3	66.32274	16.84	
^{133}Cs^2	66.45257	100.00	-----
^{133}C$^{2}_{11}$	66.50168	10.90	+1353
^{200}Hg^3	66.65611	23.13	-----
^{89}Y^{32}	66.67929	100.00	+2876
^{67}Zn	66.92714	04.11	-----
^{66}ZnH	66.93387	27.81	+9945
^{55}MnC	66.93805	98.89	+6134
^{51}VO	66.93889	99.52	+5696
^{67}S$_2$	66.93933	00.064	+5490
^{28}Si^{39}K	66.94064	85.85	+4958
^{54}Cr^{13}C	66.94222	00.026	+4438
^{54}Fe^{13}C	66.94296	00.064	+4231
^{40}Ca^{27}Al	66.94440	96.97	+3878
^{49}Ti^{18}O	66.94711	00.011	+3370
^{134}Ba^2	66.95213	02.42	+2678
^{134}Xe^2	66.95271	10.44	+2617
^{35}ClO$_2$	66.95865	75.17	+2124
^{67}CaC$_2$	66.95878	00.157	+2115
^{31}PC$_3$	66.97376	96.72	+1434
^{201}Hg^3	66.99010	13.22	+1063
^{134}C$^{2}_{11}$	67.00336	00.611	+ 878
C$_5$H$_7$	67.05474	94.49	+ 525
^{202}Hg^3	67.32354	29.80	
^{135}Ba^2	67.45278	06.59	
^{90}Zr^{32}	67.42825	51.46	
^{203}Tl^3	67.6573	29.50	
^{68}Zn	67.92486	18.57	-----
^{56}FeC	67.93194	90.64	+9594
^{67}ZnH	67.93496	04.11	+6725
^{52}CrO	67.93543	83.56	+6426
^{68}S$_2$	67.93573	00.204	+6249
^{28}SiCa	67.93979	89.42	+4550
^{55}Mn^{13}C	67.94140	01.107	+4107
^{41}KAl	67.94337	06.88	+3670
^{50}Ti^{18}O	67.94395	00.011	+3558
^{50}Cr^{18}O	67.94521	00.009	+3339
^{136}Ba^2	67.95219	07.81	+2485
^{136}Ce^2	67.95354	00.193	+2365
^{136}Xe^2	67.95360	08.87	+2363
^{28}Si$_2$C	67.95386	84.09	+2342
^{44}CaC$_2$	67.95500	02.015	+2254
^{32}SC$_3$	67.97207	91.88	+1439
^{204}Pb^3	67.99103	01.48	+1027
^{204}Hg^3	67.99116	06.85	+1025
C$_5$H$_8$	68.06256	94.48	+ 493
^{205}Tl^3	68.3246	70.50	
^{137}Ba^2	68.45279	11.32	
^{206}Pb^3	68.65815	23.6	
^{69}Ga	68.92571	60.4	-----
^{92}Zr^{32}	68.92850	17.11	+25E3
^{68}ZnH	68.93268	18.57	+9889
^{56}Fe^{13}C	68.93529	01.015	+7194
^{57}FeC	68.93541	02.166	+7106
^{53}CrO	68.93556	09.53	+6998
^{69}S$_2$	68.93855	02.E4	+5368
^{138}Ba^2	68.95244	71.66	+2579
^{138}Ce^2	68.95302	00.25	+2524
^{138}La^2	68.95337	00.089	+2487
^{69}Si$_2$C	68.95342	09.50	+2487
^{37}ClO$_2$	68.95570	24.35	+2298
^{45}ScC$_2$	68.95592	97.80	+2282
^{69}SC$_3$	68.97542	03.83	+1387
^{207}Pb^3	68.99196	22.6	+1040
C$_5$H$_9$	69.0704	94.46	+ 476
^{208}Pb^3	69.32555	52.3	
^{139}La^2	69.45302	99.911	
^{209}Bi^3	69.65978	100.00	
^{70}Ge	69.92399	20.52	-----
^{70}Ge	69.92399	20.52	-----
^{70}Zn	69.92534	00.62	+52E3
^{70}FeC	69.93331	00.35	+7503
^{69}GaH	69.93353	60.4	+7330
^{54}CrO	69.93379	02.38	+7135
^{54}FeO	69.93452	05.81	+6640
^{70}S$_2$	69.93495	00.001	+6380
^{58}NiC	69.93535	68.41	+6155
^{35}Cl$_2$	69.93771	56.05	+5097
^{57}Fe^{13}C	69.93876	00.024	+4734
^{52}Cr^{18}O	69.93967	00.171	+4451
^{70}Si$_2$C	69.95069	05.95	+2619
^{46}CaC$_2$	69.95369	00.003	+2354
^{46}TiC$_2$	69.95263	07.82	+2442
^{27}Al$_2$O	69.95799	99.76	+2058
^{70}SC$_3$	69.96786	04.10	+1592
C$_5$H$_{10}$	70.0782	94.45	+ 453
Na$_2$C$_2$	69.97976	97.80	+1254
^{94}Zr^{32}	70.43073	17.40	-----
^{141}Pr^2	70.45374	100.00	+3062
^{71}Ga	70.92482	39.6	-----
^{70}GeH	70.93181	20.52	+10E3
^{55}MnO	70.93297	99.76	+8702
^{59}CoC	70.93318	98.89	+8484
^{44}CaAl	70.93654	02.06	+6052
^{58}Fe^{13}C	70.93666	03.7E3	+5990
^{58}Ni^{13}C	70.93870	00.766	+5110
^{53}Cr^{18}O	70.93981	00.019	+4735
^{54}FeOH	70.94231	05.81	+4055
^{71}TiC$_2$	70.95176	07.31	+2633
^{39}KO$_2$	70.95351	92.65	+2472
^{142}Nd^2	70.95374	27.11	+2452
^{142}Ce^2	70.95465	11.07	+2378
^{23}NaO$_3$	70.97451	96.72	+1427
^{23}NaC$_4$	70.98978	95.65	+1091
C$_5$H$_{11}$	71.08602	94.44	+ 440
^{143}Nd^2	71.45479	12.17	
^{72}Ge	71.92159	27.43	-----
^{56}FeO	71.92685	91.44	+14E3
^{60}NiC	71.93077	25.94	+7835
^{72}SiCa	71.93193	01.93	+6956
^{71}GaH	71.93264	39.6	+6509
^{36}S$_2$	71.93418	3.0E6	+5713
^{72}Cl$_2$	71.93476	36.97	+5461
^{59}Co^{13}C	71.93653	01.107	+4814
^{54}Cr^{18}O	71.93803	00.005	+4383
^{54}Fe^{18}O	71.93877	00.012	+4179
^{72}TiC$_2$	71.94795	72.50	+2728
^{28}Si$_2$O	71.94877	84.83	+2646
^{40}CaO$_2$	71.95239	96.50	+2335
^{43}CaC$_2$	71.95253	00.181	+2325
^{144}Nd^2	71.95490	23.85	+2159
^{24}Mg$_3$	71.95513	48.74	+2144
^{144}Sm^2	71.95583	03.09	+2101
^{24}MgO$_3$	71.96977	78.15	+1493
^{24}Mg$_2$C$_2$	71.97003	60.58	+1485
^{24}MgC$_4$	71.98504	75.27	+1134
^{72}C$_6$	72.00000	93.52	+ 917
^{145}Nd^2	72.45603	08.30	-----
^{145}C$^{2}_{12}$	72.50168	11.76	+1587
^{73}Ge	72.92334	07.76	-----
^{72}GeH	72.92941	27.43	+12E3
^{57}FeO	72.93032	02.19	+10E3
^{73}NiC	72.93109	01.47	+9409
^{56}FeOH	72.93464	91.45	+6453
^{55}Mn^{18}O	72.93721	00.204	+5261
^{73}TiC$_2$	72.94787	07.01	+2973
^{73}Si$_2$O	72.94833	08.64	+2918
^{41}KO$_2$	72.95163	06.85	+2578
^{73}Mg$_3$	72.95592	18.32	+2238
^{146}Nd^2	72.95635	17.22	+2209
^{37}ClC$_3$	72.96590	23.67	+1713
^{25}MgO$_3$	72.97057	10.06	+1544
^{73}Mg$_2$C$_2$	72.97088	16.96	+1534
^{73}MgC$_4$	72.98584	13.07	+1167
^{73}C$_6$	73.00336	06.29	+ 911
^{12}C$_6$H	73.00782	93.51	+ 863
^{147}Sm^2	73.45725	14.97	
^{74}Ge	73.92100	36.54	-----
^{74}Se	73.92254	00.87	+48E3
^{58}FeO	73.92822	00.33	+10E3
^{74}NiC	73.92834	03.63	+10E3
^{58}NiO	73.93026	69.01	+7983
^{56}Fe^{18}O	73.93110	00.187	+7319
^{73}GeH	73.93116	07.76	+7276
^{37}Cl$_2$	73.93181	05.99	+6838
^{39}KCl	73.93256	70.92	+6395
^{57}FeOH	73.93814	02.19	+4323
^{50}CrC$_2$	73.94065	04.22	+3762
^{74}TiC$_2$	73.94479	05.34	+3107
^{58}Si$_2$O	73.94560	05.91	+3005
^{42}CaO$_2$	73.94843	00.64	+2695
^{74}Mg$_3$	73.95268	23.18	+2333
^{148}Sm^2	73.95721	11.24	+2041
^{148}Nd^2	73.95823	05.73	+1986
^{26}MgO$_3$	73.96732	11.09	+1597
^{74}Mg$_2$C$_2$	73.96763	18.54	+1585
^{74}MgC$_4$	73.98259	11.11	+1200
^{74}C$_6$	74.00670	00.176	+ 863
^{12}C$_6$H$_2$	74.01564	93.50	+ 781
^{149}Sm^2	74.45840	13.83	
^{75}As	74.92171	100.00	-----
^{59}CoO	74.92809	99.76	+12E3
^{74}GeH	74.92882	36.53	+11E3
^{48}TiAl	74.92949	73.98	+9630
^{63}CuC	74.92959	68.33	+9506
^{74}SeH	74.93036	00.87	+8661
^{57}Fe^{18}O	74.93457	00.004	+5812
^{51}VC$_2$	74.94398	97.56	+3364
^{75}Mg$_3$	74.95347	05.34	+2359
^{25}Mg$_3$	74.95752	00.01	+2092
^{150}Sm^2	74.95845	07.44	+2039
^{43}CaO$_2$	74.95858	00.145	+2032
^{150}Nd^2	74.96041	05.63	+1936
^{39}KC$_3$	74.96371	90.04	+1784
^{27}AlO$_3$	74.96627	99.28	+1681
^{27}AlC$_4$	74.98154	95.65	+1253
C$_6$H$_3$	75.02346	93.48	+ 736
^{151}Eu^2	75.45977	47.32	
^{76}Se	75.91928	09.02	-----
^{76}Ge	75.92019	07.76	+38E3
^{60}NiO	75.92568	26.17	+12E3
^{64}NiC	75.92796	01.07	+8746
^{64}ZnC	75.92914	48.35	+7700
^{75}AsH	75.92953	99.985	+7407
^{76}KCl	75.92961	27.98	+7349
^{63}Cu^{13}C	75.93292	00.765	+5566
^{52}CrC$_2$	75.94051	81.92	+3576
^{32}S$_2$C	75.94414	89.25	+3054
^{44}CaO$_2$	75.94529	02.05	+2919
^{76}Mg$_3$	75.95023	03.29	+2453
^{152}Sm^2	75.95968	26.72	+1879
^{152}Gd^2	75.95971	00.20	+1878
^{28}SiO$_3$	75.96166	91.54	+1791
^{40}CaC$_3$	75.96259	93.79	+1753
^{28}SiC$_4$	75.97693	88.19	+1318
^{12}CO$_4$	75.97964	97.94	+1259
^{12}C$_6$H$_4$	76.03128	93.47	+ 678
^{153}Eu^2	76.4603	52.18	
^{77}Se	76.91998	07.58	-----
^{61}NiO	76.92600	01.19	+13E3
^{76}SeH	76.92710	09.02	+11E3
^{65}CuC	76.92778	30.57	+9862
^{76}GeH	76.92801	07.76	+9579
^{65}CuC	76.92778	30.57	+9862
^{64}Zn^{13}C	76.93131	00.54	+6789
^{53}CrC$_2$	76.94065	09.34	+3721
^{52}Cr^{25}C$_2$	76.94387	01.33	+3220
^{45}ScO$_2$	76.94752	99.52	+2793
^{77}Mg$_3$	76.95102	00.38	+2478
^{154}Gd^2	76.96047	02.15	+1900
^{154}Sm^2	76.96097	22.71	+1877
^{29}SiO$_3$	76.96122	04.67	+1865
^{41}KC$_3$	76.96183	06.65	+1833
^{77}SiC$_4$	76.97649	08.46	+1361
^{13}CO$_4$	76.98300	01.10	+1221
^{12}C$_6$H$_5$	77.03910	93.46	+ 646
^{232}Th^3	77.3460	100.00	
^{155}Gd^2	77.4614	14.73	
^{78}Se	77.91739	23.52	-----
^{78}Kr	77.92019	00.354	+28E3
^{62}NiO	77.92325	03.64	+13E3
^{66}ZnC	77.92605	27.50	+8997
^{39}K$_2$	77.92742	86.68	+7768
^{41}K^{37}Cl	77.92773	01.68	+7536
^{77}SeH	77.92780	07.58	+7485
^{65}Cu^{13}C	77.93113	00.34	+5671
^{78}CrC$_2$	77.93887	02.54	+3627
^{54}FeC$_2$	77.93961	05.69	+3507
^{78}S$_2$C	77.93993	07.95	+3457
^{46}TiO$_2$	77.94243	07.96	+3112
^{78}Mg$_3$	77.94777	00.14	+2566
^{156}Dy^2	77.957/	00.052	+1967

$^{30}SiO_3$	77.95849	03.07	+1895
$^{42}CaC_3$	77.95863	00.62	+1889
$^{156}Gd^2$	77.96113	20.47	+1781
$^{31}P_2O$	77.96244	99.76	+1730
$^{27}Al_2C_2$	77.96308	97.80	+1705
$^{23}Na_2O_2$	77.96938	97.52	+1499
$^{78}SiC_4$	77.97376	03.16	+1382
$^{14}NO_4$	77.98271	98.67	+1193
$^{12}C^{2}_{13}$	78.00000	86.49	+ 943
$^{12}C_6H_6$	78.04692	93.45	+ 602
$^{235}U^3$	78.3476	00.72	
$^{157}Gd^2$	78.4621	15.68	-----
$^{157}C^{2}_{13}$	78.50168	12.60	+1982
^{79}Br	78.91839	50.537	-----
$^{52}CrAl$	78.92205	83.76	+22E3
^{63}CuO	78.92451	68.92	+13E3
^{78}SeH	78.92521	23.52	+12E3
^{79}ZnC	78.92714	04.42	+9019
$^{79}K_2$	78.92771	00.022	+8468
$^{66}Zn^{13}C$	78.92941	00.31	+7168
$^{55}MnC_2$	78.93805	97.80	+4014
$^{47}TiO_2$	78.94156	07.25	+3406
$^{31}PO_3$	78.95849	99.28	+1968
$^{79}CaC_3$	78.95878	00.161	+1954
$^{158}Dy^2$	78.96200	00.09	+1810
$^{158}Gd^2$	78.9622	24.87	+1801
$^{31}PC_4$	78.97376	95.65	+1425
$^{158}C^{2}_{13}$	79.00335	00.847	+ 929
C_6H_7	79.05474	93.44	+ 579
$^{238}U^3$	79.3495	99.274	-----
$^{159}Tb^2$	79.46244	100.000	+ 703
^{80}Se	79.91647	49.82	-----
^{80}Kr	79.91659	02.27	+67E4
$^{28}Si^{52}Cr$	79.91744	77.24	+82E3
^{64}NiO	79.92287	01.08	+13E3
^{64}ZnO	79.92405	48.77	+11E3
^{80}ZnC	79.92486	18.41	+9525
$^{40}Ca_2$	79.92517	93.45	+9186
$^{80}K_2$	79.92554	12.81	+8811
$H^{79}Br$	79.92622	50.52	+8197
$^{56}FeC_2$	79.93194	89.64	+5166
$^{55}Mn^{25}C_2$	79.94141	02.19	+3204
$^{48}TiO_2$	79.93775	73.62	+3755
$^{32}S_2O$	79.93905	90.03	+3539
$^{48}CaO_2$	79.94233	00.184	+3090
$^{28}Si_2C_2$	79.95386	83.16	+2137
$^{44}CaC_3$	79.95500	01.99	+2074
$^{32}SO_3$	79.95602	94.32	+1981
$^{24}Mg_2O_2$	79.95990	61.64	+1840
$^{160}Dy^2$	79.9620	02.294	+1755
$^{160}Gd^2$	79.96361	21.90	+1695
$^{32}SC_4$	79.97207	92.77	+1437
$^{12}C_6H_8$	80.06256	93.43	+ 547
$^{161}Dy^2$	80.4629	18.88	
^{81}Br	80.91642	49.463	-----
$^{54}FeAl$	80.92115	05.82	+17E3
^{65}CuO	80.92269	30.84	+13E3
^{80}SeH	80.92429	49.81	+10E3
^{69}GaC	80.92571	59.73	+8710
$^{81}FeC_2$	80.93541	04.15	+4261
$^{49}TiO_2$	80.93767	05.48	+3808
$^{27}Al_3$	80.94462	100.00	+2869
$^{81}Si_2C_2$	80.95342	12.12	+2187
$^{49}Mg_2O_2$	80.96070	15.87	+1827
$^{162}Dy^2$	80.9628	25.53	+1745
$^{162}Er^2$	80.96436	00.136	+1688
$^{12}C_6H_9$	81.07038	93.41	+ 526
$^{163}Dy^2$	81.4639	24.97	
^{82}Kr	81.91345	11.56	-26E3
$^{28}Si^{54}Fe$	81.91654	05.37	-91E4
^{82}Se	81.91663	09.19	-----
$^{55}MnAl$	81.91959	100.00	+28E3
^{66}ZnO	81.92096	27.74	+19E3
$^{82}Ca_2$	81.92121	01.24	+18E3
$^{41}K_2$	81.92366	00.47	+12E3
^{70}GeC	81.92399	20.29	+11E3
$H^{81}Br$	81.92425	49.44	+11E3
^{70}ZnC	81.92534	00.63	+9405
$^{69}Ga^{13}C$	81.92906	00.669	+6590
$^{82}FeC_2$	81.93331	00.368	+4911
$^{50}TiO_2$	81.93459	05.31	+4561
$^{58}NiC_2$	81.93535	67.66	+4376
$^{66}S_2O$	81.93484	08.00	+4498
$^{50}CrO_2$	81.93585	04.29	+4262
$^{82}Si_2C_2$	81.95069	05.98	+2405
$^{34}SO_3$	81.95261	04.19	+2277
$^{46}TiC_3$	81.95263	07.74	+2275
$^{50}Mg_2O_2$	81.95745	18.53	+2007
$^{164}Dy^2$	81.9643	28.18	+1718
$^{164}Er^2$	81.9649	01.56	+1697
$^{34}SC_4$	81.96786	04.04	+1599
$^{165}Ho^2$	82.46455	100.00	
$^{56}FeAl$	82.91348	91.66	-15E4
^{83}Kr	82.91405	11.55	-----
$^{28}Si^{55}Mn$	82.91498	92.21	+89E3
^{67}ZnO	82.92205	04.10	+10E3
$^{83}Ca_2$	82.92278	00.28	+9498
^{82}SeH	82.92445	09.19	+7973
^{71}GaC	82.92482	39.16	+7699
$^{59}CoC_2$	82.93318	97.80	+4334
$^{51}VO_2$	82.93378	99.28	+4202
$^{83}TiC_3$	82.95176	07.31	+2199
$^{35}ClO_3$	82.95355	74.98	+2099
$^{166}Er^2$	82.9644	33.41	+1647
$^{35}ClC_4$	82.96885	72.24	+1513
$^{167}Er^2$	83.4653	22.94	
$^{28}Si^{56}Fe$	83.90887	84.52	-19E3
^{84}Kr	83.91325	56.90	-48E3
^{84}Sr	83.91325	00.56	-----
$^{57}FeAl$	83.91695	02.19	+23E3
$^{84}Ca_2$	83.91808	03.98	+17E3
^{68}ZnO	83.91977	18.53	+13E3
^{72}GeC	83.92159	27.13	+10E3
$^{52}CrO_2$	83.93031	83.36	+4919
$^{28}Si_3$	83.93079	78.40	+4784
$^{60}NiC_2$	83.93078	25.65	+4787
$^{84}TiC_3$	83.94795	71.79	+2418
$^{48}CaC_3$	83.95253	00.18	+2136
$^{168}Er^2$	83.9654	27.07	+1609
$^{168}Yb^2$	83.96695	00.135	+1563
$^{12}C_7$	84.00000	92.48	+ 967
$^{169}Tm^2$	84.46717	100.00	-----
$^{169}C^{2}_{14}$	84.50168	13.42	+2448
$^{85}SiFe$	84.90843	06.33	-24E3
^{85}Rb	84.91202	72.15	-----
$^{58}FeAl$	84.91485	00.33	+30E3
^{84}SrH	84.92107	00.56	+9383
^{85}GeC	84.92334	07.97	+7501
$^{85}Si_3$	84.93035	11.99	+4632
$^{53}CrO_2$	84.93045	09.50	+4607
$^{85}NiC_2$	84.93109	01.73	+4453
$^{85}TiC_3$	84.94787	07.73	+2369
$^{37}ClC_4$	84.96590	02.40	+1576
$^{170}Yb^2$	84.967/	03.03	+1544
$^{170}Er^2$	84.9678	14.88	+1522
$^{85}C_7$	85.00336	07.25	+ 930
$^{12}C_7H$	85.00782	92.49	+ 886
$^{171}Yb^2$	85.468/	14.31	
^{86}Sr	85.90935	09.86	-----
^{86}Kr	85.91079	17.37	+60E3
$^{54}Fe^{32}S$	85.91168	05.53	+37E3
^{70}GeO	85.91390	60.3	+8996
^{85}RbH	85.91984	72.14	+8190
^{70}ZnO	85.92025	00.62	+7832
^{86}GeC	85.92100	36.23	+7374
^{74}SeC	85.92254	00.87	+6513
$^{86}Si_3$	85.92762	08.49	+4702
$^{62}NiC_2$	85.92834	03.58	+4524
$^{54}CrO_2$	85.92867	02.37	+4446
$^{54}FeO_2$	85.92941	05.79	+4283
$^{86}TiC_3$	85.94479	05.34	+2424
$^{50}CrC_3$	85.94065	04.17	+2341
$^{27}Al_2O_2$	85.95289	99.52	+1973
$^{172}Yb^2$	85.9626	21.82	+1612
$^{31}P_2C_2$	85.96753	97.80	+1477
$^{86}C_7$	86.00670	00.244	+ 882
$^{12}C_7H_2$	86.01564	92.48	+ 808
$^{173}Yb^2$	86.469/	16.13	
^{87}Sr	86.90899	07.02	-----
^{87}Rb	86.90930	27.85	+28E4
^{86}SrH	86.91717	09.86	+11E3
^{71}GaO	86.91973	39.50	+8092
^{75}AsC	86.92171	98.89	+6832
$^{74}Ge^{13}C$	86.92436	00.40	+5654
$^{55}MnO_2$	86.92785	99.52	+4608
$^{87}Si_3$	86.92718	00.81	+4773
$^{39}KO_3$	86.94841	92.43	+2205
$^{174}Yb^2$	86.9628/	31.84	+1615
$^{39}KC_4$	86.96371	89.05	+1588
$^{174}Hf^2$	86.9707	00.18	+1425
$^{12}C_7H_3$	87.02346	92.47	+ 759
$^{175}Lu^2$	87.471/	97.41	
$^{56}Fe^{32}S$	87.90401	87.08	-44E3
^{88}Sr	87.90601	82.56	-----
$^{40}Ca^{48}Ti$	87.91081	71.74	+18E3
^{72}GeO	87.91650	27.37	+8372
$^{88}Ca_2$	87.91653	00.40	+8348
^{87}SrH	87.91681	07.02	+8139
^{87}RbH	87.91712	27.85	+7912
^{76}SeC	87.91928	08.92	+6624
^{76}GeC	87.92129	07.67	+5753
$^{56}FeO_2$	87.92174	91.22	+5585
$^{88}Si_3$	87.92445	00.28	+4767
$^{64}ZnC_2$	87.92914	47.81	+3801
$^{64}NiC_2$	87.92796	01.06	+4003
$^{52}CrC_3$	87.94051	81.01	+2547
$^{28}Si_2O_2$	87.94368	84.62	+2333
$^{32}S_2C_2$	87.94414	88.26	+2305
$^{40}CaO_3$	87.94759	96.27	+2114
$^{40}CaC_4$	87.96286	92.75	+1546
$^{24}MgO_4$	87.96468	77.94	+1498
$^{176}Hf^2$	87.9704	05.20	+1365
$^{176}Lu^2$	87.9710	02.59	+1352
$^{176}Yb^2$	87.97136	12.73	+1345
$^{12}C_7H_4$	88.03128	92.46	+ 702
$^{177}Hf^2$	88.4713	18.50	
^{89}Y	88.90572	100.00	-----
$^{57}Fe^{32}S$	88.90748	02.08	+51E3
^{88}SrH	88.91383	82.55	+11E3
^{73}GeO	88.91825	07.73	+7095
^{89}SeC	88.91998	07.60	+6235
$^{89}Si_3$	88.92401	00.013	+4861
$^{57}FeO_2$	88.92521	02.18	+4562
$^{65}CuC_2$	88.92778	30.23	+4030
$^{89}CrC_3$	88.94065	11.96	+2545
$^{89}Si_2O_2$	88.94324	08.62	+2370
$^{41}KO_3$	88.94563	06.83	+2228
$^{41}KC_4$	88.96183	06.58	+1584
$^{25}MgO_4$	88.96548	10.03	+1488
$^{178}Hf^2$	88.9715	27.14	+1352
$^{12}C_7H_5$	89.03910	92.45	+ 667
$^{179}Hf^2$	89.4726	13.75	
^{90}Zr	89.90433	51.46	-----
$^{45}Sc_2$	89.91184	100.00	+12E3
^{89}YH	89.91354	99.985	+9762
^{74}GeO	89.91591	36.38	+7764
^{90}SeC	89.91739	23.32	+6884
^{74}SeO	89.91745	00.87	+6852
$^{58}FeO_2$	89.92311	00.32	+4787
$^{58}NiO_2$	89.92515	68.85	+4318
$^{66}ZnC_2$	89.92605	27.20	+4139
$^{39}K_2C$	89.92742	85.72	+3894
$^{90}CrC_3$	89.93887	02.61	+2602
$^{54}FeC_3$	89.93961	05.63	+2548
$^{90}Si_2O_2$	89.94051	05.89	+2485
$^{26}MgO_4$	89.96223	11.06	+1553
$^{27}Al_2C_3$	89.96308	96.72	+1530
$^{180}W^2$	89.9723	00.135	+1323
$^{180}Ta^2$	89.973/	00.012	+1309
$^{180}Hf^2$	89.9731	35.24	+1307
$^{12}C^{2}_{15}$	90.00000	84.58	+ 940
$^{12}C_7H_6$	90.04692	92.43	+ 631
$^{181}Ta^2$	90.4729	99.988	-----
$^{181}C^{2}_{15}$	90.50168	14.22	+3144
^{91}Zr	90.90532	11.22	-----
^{90}ZrH	90.91215	51.45	+13E3
^{75}AsO	90.91662	99.76	+8045
^{79}BrC	90.91839	49.98	+6955
$^{59}CoC_2$	90.92298	97.80	+5148
$^{91}ZnC_2$	90.92714	04.63	+4166
$^{55}MnC_3$	90.93805	96.72	+2777
$^{54}Fe^{37}C_3$	90.94297	00.189	+2414
$^{27}AlO_4$	90.96114	99.04	+1629
$^{182}W^2$	90.9730	26.41	+1343
$^{182}C^{2}_{15}$	91.00335	01.115	+ 927
$^{183}W^2$	91.4741	14.40	
$^{40}Ca^{52}Cr$	91.90337	81.22	-71E3
^{92}Zr	91.90467	17.11	-----
$^{46}Ti_2$	91.90526	00.64	+16E4
^{92}Mo	91.90855	15.84	+24E3
^{91}ZrH	91.91314	11.22	+11E3
^{76}SeO	91.91419	09.01	+9654
^{76}GeO	91.91620	07.75	+7971
^{80}SeC	91.91647	49.27	+7789
$^{60}NiO_2$	91.92057	26.10	+5780
$^{92}ZnC_2$	91.92486	18.25	+4552

$^{40}Ca_2C$	91.92517	92.42	+4483
$^{44}CaO_3$	91.94023	02.05	+2584
$^{28}Si_2C_3$	91.95386	82.24	+1868
$^{44}CaC_4$	91.95550	01.97	+1808
$^{28}SiO_4$	91.95657	91.32	+1771
$^{184}Os^{2}$	91.973	00.018	+1345
$^{184}W^{2}$	91.9745	30.64	+1316
$^{185}Re^{2}$	92.474	37.07	
^{93}Nb	92.90566	100.00	-----
^{92}ZrH	92.91249	17.11	+14E3
^{77}SeO	92.91489	07.57	+10E3
^{81}BrC	92.91642	48.92	+8634
$^{61}NiO_2$	92.92089	01.18	+6100
$^{69}GaC_2$	92.92571	59.07	+4634
$^{93}FeC_3$	92.93530	05.10	+3134
$^{27}Al_3C$	92.94462	98.89	+2385
$^{31}P_3$	92.95129	100.00	+2036
$^{93}Si_2C_3$	92.95342	11.14	+1945
$^{29}SiO_4$	92.95613	04.65	+1841
$^{186}W^{2}$	92.9754	28.41	+1332
$^{186}Os^{2}$	92.976/	01.59	+1321
$^{187}Re^{2}$	93.477/	62.93	-----
$^{187}Os^{2}$	93.478/	01.64	+94E3
$^{94}Ti_2$	93.90058	12.37	-13E3
$^{40}CaFe$	93.90247	05.64	-18E3
^{94}Mo	93.90594	09.04	-55E3
^{94}Zr	93.90764	17.40	-----
^{78}SeO	93.91230	23.47	+20E3
^{93}NbH	93.91348	99.985	+16E3
^{82}SeC	93.91663	09.09	+10E3
$^{62}NiO_2$	93.91814	03.64	+8944
$^{39}K_2O$	93.92233	86.47	+6393
$^{70}GeC_2$	93.92399	20.07	+5744
$^{94}FeC_3$	93.93331	00.39	+3658
$^{58}NiC_3$	93.93535	66.91	+3389
$^{46}TiO_3$	93.93736	07.94	+3160
$^{94}Si_2C_3$	93.95069	06.01	+2181
$^{46}TiC_4$	93.95263	07.65	+2087
$^{30}SiO_4$	93.95340	03.06	+2052
$^{31}P_2O_2$	93.95735	99.52	+1890
$^{188}Os^{2}$	93.9785/	13.3	+1325
$^{189}Os^{2}$	94.4793/	16.1	
$^{95}Ti_2$	94.89970	11.67	-20E3
$^{40}CaMn$	94.90091	96.97	-27E3
^{95}Mo	94.90444	15.72	-----
^{79}BrC	94.91330	50.42	+11E3
^{94}MoH	94.91376	09.04	+10E3
^{94}ZrH	94.91546	17.40	+8612
$^{40}CaFe$	95.89480	88.88	-6614
$^{96}Ti_2$	95.89589	56.38	-7152
^{96}Mo	95.90496	16.53	-22E3
^{96}Ru	95.9087	05.51	-16E4
^{96}Zr	95.90930	02.80	-----
^{80}SeO	95.91138	49.71	+46E3
^{95}MoH	95.91226	15.72	+32E3
^{84}SrC	95.91325	00.55	+24E3
$^{32}S_3$	95.91622	85.74	+14E3
$^{64}NiO_2$	95.91776	01.07	+11E3
$^{64}ZnO_2$	95.91896	48.65	+9928
$^{40}Ca_2O$	95.92008	93.22	+8897
$^{72}GeC_2$	95.92159	26.83	+7804
$^{60}NiC_3$	95.93077	25.40	+4467
$^{28}Si_3C$	95.93079	77.53	+4463
$^{48}TiO_3$	95.93265	73.45	+4107
$^{32}S_2O_2$	95.93396	89.82	+3889
$^{48}TiC_4$	95.94795	71.07	+2481
$^{32}SO_4$	95.95173	94.09	+2260
$^{192}Os^{2}$	95.9811/	41.0	+1336
$^{192}Pt^{2}$	95.9824/	00.78	+1312
$^{12}C_8$	96.00000	91.46	+1057
$^{193}Ir^{2}$	96.4834/	62.7	-----
$^{193}C^{2}_{16}$	96.50168	14.99	+5278
$^{97}Ti_2$	96.89581	08.93	-9318
$^{40}CaFe$	96.89827	02.12	-12E3
^{97}Mo	96.90621	09.46	-----
^{81}BrO	96.91133	49.34	+19E3
^{85}RbC	96.91202	71.35	+17E3
^{96}MoH	96.91278	16.53	+15E3
$^{97}S_3$	96.91561	02.06	+10E3

^{96}ZrH	96.91712	02.80	+8882
$^{65}CuO_2$	96.91758	30.76	+8523
$^{97}GeC_2$	96.92334	08.19	+5657
$^{97}Si_3C$	96.93035	12.73	+4014
$^{97}NiC_3$	96.93109	02.00	+3895
$^{49}TiO_3$	96.93257	05.47	+3676
$^{27}Al_3O$	96.93953	99.76	+2908
$^{97}TiC_4$	96.94787	08.44	+2326
$^{194}Pt^{2}$	96.9817/	32.9	+1284
$^{194}C^{2}_{16}$	97.00335	01.26	+ 998
$^{97}C_8$	97.00335	08.20	+ 998
$^{12}C_8H$	97.00782	91.45	+ 954
$^{195}Pt^{2}$	97.4831/	33.8	
$^{98}Ti_2$	97.89273	08.20	-7389
^{98}Mo	97.90598	23.78	-----
^{86}SrC	97.90935	09.75	+29E3
^{82}SeO	97.91154	09.18	+18E3
^{97}MoH	97.91403	09.46	+12E3
$^{98}S_3$	97.91201	11.43	+16E3
$^{85}Rb^{13}C$	97.91545	00.80	+10E3
$^{66}ZnO_2$	97.91585	27.68	+9920
$^{98}GeC_2$	97.92100	35.91	+6518
$^{74}SeC_2$	97.92254	00.85	+5912
$^{98}Si_3C$	97.92762	08.53	+4524
$^{98}NiC_3$	97.92834	03.58	+4379
$^{50}TiO_3$	97.92952	05.30	+4159
$^{50}CrO_3$	97.93078	04.28	+3948
$^{98}TiC_4$	97.94479	05.35	+2523
$^{50}CrC_4$	97.94605	04.12	+2443
$^{34}SO_4$	97.94752	04.18	+2357
^{98}Ru	97.954/	01.87	+2039
$^{31}P_2C_3$	97.96753	96.72	+1591
$^{196}Hg^{2}$	97.98291	00.146	+1273
$^{196}Pt^{2}$	97.9836	25.3	+1261
$^{98}C_8$	98.00670	00.321	+ 972
$^{12}C_8H_2$	98.01564	91.44	+ 893
$^{197}Au^{2}$	98.4836	100.00	
$^{99}Ti_2$	98.89266	00.59	-7387
^{99}Ru	98.90605	12.72	-----
^{99}SrC	98.90899	07.05	+34E3
^{87}RbC	98.90930	27.54	+30E3
^{98}MoH	98.91380	23.78	+13E3
$^{67}ZnO_2$	98.91694	04.09	+9082
$^{75}AsC_2$	98.92171	97.80	+6316
$^{63}CuC_3$	98.92959	66.82	+4202
$^{35}ClO_4$	98.94849	74.80	+2330
$^{198}Pt^{2}$	98.9823	07.21	+1297
$^{198}Hg^{2}$	98.98337	10.02	+1279
C_8H_3	99.02346	91.43	+ 842
$^{199}Hg^{2}$	99.48411	16.84	
$^{50}Ti_2$	99.88958	00.29	-5905
$^{50}Cr_2$	99.89210	00.19	-6933
^{100}Ru	99.905/	12.62	-67E3
^{100}SrC	99.90610	81.73	-25E4
^{100}Mo	99.90651	09.63	-----
^{84}SrO	99.90816	00.56	+60E3
$^{87}Rb^{13}C$	99.91265	27.54	+16E3
$^{68}ZnO_2$	99.91466	18.43	+12E3
$^{76}SeC_2$	99.91928	08.32	+7324
$^{76}GeC_2$	99.92129	07.59	+6760
$^{52}CrO_3$	99.92521	83.16	+5340
$^{29}Si_3O$	99.92570	78.21	+5203
$^{39}K_2C_2$	99.92742	84.77	+4778
$^{64}NiC_3$	99.92796	01.04	+4655
$^{64}ZnC_3$	99.92914	47.28	+4415
$^{52}CrC_4$	99.94051	80.11	+2938
$^{32}S_2C_3$	99.94414	87.29	+2654
$^{200}Hg^{2}$	99.98416	23.13	+1286
C_8H_4	100.03128	91.42	+ 801
$^{201}Hg^{2}$	100.48515	13.22	
^{101}Ru	100.905/	17.07	-----
^{89}YC	100.90572	98.89	+14E4
^{85}RbO	100.90693	71.93	+52E3
$^{88}Sr^{13}C$	100.90945	00.914	+23E3
^{100}MoH	100.91433	09.63	+11E3
$^{69}GaO_2$	100.91551	60.11	+9601
$^{101}SeC_2$	100.91998	07.61	+6736
$^{101}Si_3O$	100.92526	11.96	+4981

$^{53}CrO_3$	100.92538	09.48	+4951
$^{65}CuC_3$	100.92778	29.89	+4430
$^{101}CrC_4$	100.94065	12.72	+2830
$^{202}Hg^{2}$	100.98531	29.80	+1256
C_8H_5	101.03910	91.42	+ 752
$^{135}Ba^{32}$	101.17916	06.59	
$^{203}Tl^{2}$	101.4860	29.50	
$^{102}Cr_2$	101.88656	07.22	-5935
$^{51}V_2$	101.88795	99.52	-6458
^{102}Ru	101.90373	31.61	-----
^{86}SrO	101.90426	09.84	+19E4
^{90}ZrC	101.90433	50.89	+17E4
^{102}Pd	101.90486	00.96	+90E3
$^{89}Y^{13}C$	101.90907	01.107	+19E3
$^{70}GeO_2$	101.91379	20.42	+10E3
$^{102}SeC_2$	101.91739	23.15	+7460
$^{102}Si_3O$	101.92253	08.47	+5420
$^{54}CrO_3$	101.92360	02.36	+5129
$^{54}FeO_3$	101.92434	05.78	+4944
$^{66}ZnC_3$	101.92605	26.90	+4566
$^{136}Ba^{32}$	101.92828	07.81	+4151
$^{102}CrC_4$	101.93877	02.69	+2900
$^{54}FeC_4$	101.93961	05.57	+2840
$^{27}Al_2O_3$	101.94781	99.28	+2312
$^{204}Pb^{2}$	101.98654	01.48	+1231
$^{204}Hg^{2}$	101.98674	06.85	+1228
$^{12}C^{2}_{17}$	102.00000	82.72	+1059
C_8H_6	102.04692	91.41	+ 712
$^{205}Tl^{2}$	102.4869	70.50	-----
$^{205}C^{2}_{17}$	102.50168	15.75	+6934
$^{137}Ba^{32}$	102.67918	11.32	
$^{103}Cr_2$	102.88670	00.82	-5765
^{87}SrO	102.90390	07.00	-16E4
^{87}RbO	102.90421	27.78	-30E4
^{103}Rh	102.90455	100.00	-----
^{103}ZrC	102.90532	11.67	+13E4
$^{71}GaO_2$	102.91462	39.41	+10E3
$^{79}BrC_2$	102.91839	49.42	+7435
$^{55}MnO_3$	102.92278	99.28	+5645
$^{103}ZnC_3$	102.92714	04.88	+4555
$^{55}MnC_4$	102.93805	95.65	+3072
$^{39}KO_4$	102.94335	92.21	+2652
$^{206}Pb^{2}$	102.98722	23.6	+1245
C_8H_7	103.05474	91.40	+ 685
$^{207}Pb^{2}$	103.48794	22.6	-----
$^{138}Ba^{32}$	103.42866	71.66	1746
$^{104}Cr_2$	103.88102	70.37	-4668
^{88}SrO	103.90101	82.36	-46E3
^{104}Pd	103.90328	10.97	-----
^{104}Ru	103.90422	18.58	+11E4
^{104}ZrC	103.90467	17.04	+75E3
^{92}MoC	103.90855	15.66	+20E3
$^{72}GeO_2$	103.91139	27.30	+13E3
$^{80}SeC_2$	103.91647	48.72	+7877
$^{56}FeO_3$	103.91664	91.00	+7777
$^{104}ZnC_3$	103.92436	18.00	+4815
$^{40}Ca_2C_2$	103.92517	91.39	+4747
$^{56}FeC_4$	103.93194	87.67	+3625
$^{28}Si_2O_3$	103.93859	84.42	+2943
$^{40}CaO_4$	103.94250	96.04	+2649
$^{208}Pb^{2}$	103.98833	52.3	+1222
C_8H_8	104.06256	91.39	+ 652
$^{139}La^{32}$	104.17952	99.911	
$^{209}Bi^{2}$	104.48967	100.000	
$^{105}Cr_2$	104.88159	16.00	-4516
^{89}YO	104.90063	99.76	-25E3
^{105}Pd	104.90482	22.23	-----
^{93}NbC	104.90566	98.89	+13E4
$^{73}GeO_2$	104.91314	07.72	+13E3
$^{81}BrC_2$	104.91642	48.37	+9044
$^{57}FeO_3$	104.92011	02.17	+6861
$^{140}Ce^{32}$	104.92896	88.48	+4346
$^{105}FeC_4$	104.93541	06.02	+3429
$^{57}Si_2O_3$	104.93815	08.60	+3147
$^{27}Al_3C_2$	104.94462	97.80	+2636
$^{106}Cr_2$	105.87938	04.90	-4501
^{90}ZrO	105.89924	51.34	-29E3
^{106}Pd	105.90291	27.33	-----

$^{106}\mathrm{Pd}$	105.90291	27.33	-----
$^{106}\mathrm{Cd}$	105.90593	01.215	+35E3
$^{94}\mathrm{MoC}$	105.90594	08.94	+35E3
$^{94}\mathrm{ZrC}$	105.90764	17.21	+22E3
$^{93}\mathrm{Nb}^{13}\mathrm{C}$	105.90901	01.107	+17E3
$^{106}\mathrm{FeC_4}$	105.93331	00.41	+3484
$^{58}\mathrm{NiC_4}$	105.93525	66.17	+3265
$^{58}\mathrm{Si_2O_3}$	105.93542	05.88	+3258
$^{107}\mathrm{Cr_2}$	106.87592	00.46	-4224
$^{91}\mathrm{ZrO}$	106.90023	11.20	-23E3
$^{107}\mathrm{MoC}$	106.90444	10.68	-27E4
$^{107}\mathrm{Ag}$	106.90483	51.35	-----
$^{94}\mathrm{Zr}^{13}\mathrm{C}$	106.91099	00.193	+17E3
$^{75}\mathrm{AsO_2}$	106.91151	99.52	+16E3
$^{54}\mathrm{Cr_2}$	107.87774	00.06	-4194
$^{54}\mathrm{Fe_2}$	107.87922	00.34	-4450
$^{92}\mathrm{ZrO}$	107.89958	17.07	-28E3
$^{92}\mathrm{MoO}$	107.90346	15.80	-10E6
$^{108}\mathrm{Pd}$	107.90347	26.71	-----
$^{108}\mathrm{Cd}$	107.90407	00.875	+18E4
$^{108}\mathrm{MoC}$	107.90496	16.47	+72E3
$^{96}\mathrm{RuC}$	107.9087	05.45	+21E3
$^{76}\mathrm{SeO_2}$	107.90910	08.98	+19E3
$^{96}\mathrm{ZrC}$	107.90930	02.77	+19E3
$^{76}\mathrm{GeO_2}$	107.91111	07.72	+14E3
$^{84}\mathrm{SrC_2}$	107.91325	00.55	+11E3
$^{27}\mathrm{Al_4}$	107.92613	100.00	+4762
$^{60}\mathrm{NiC_4}$	107.93077	25.09	+3953
$^{28}\mathrm{Si_3C_2}$	107.93079	76.67	+3950
$^{44}\mathrm{CaO_4}$	107.93514	02.04	+3411
$^{12}\mathrm{C_9}$	108.00000	90.44	+1118
$^{217}\mathrm{C^2_{18}}$	108.50168	16.50	
$^{93}\mathrm{NbO}$	108.90057	99.76	-27E3
$^{109}\mathrm{Ag}$	108.90461	48.65	-----
$^{109}\mathrm{MoC}$	108.90621	09.54	+68E3
$^{77}\mathrm{SeO_2}$	108.90980	07.54	+21E3
$^{85}\mathrm{RbC_2}$	108.91202	70.56	+15E3
$^{96}\mathrm{Zr}^{13}\mathrm{C}$	108.91265	00.031	+14E3
$^{109}\mathrm{Si_3C_2}$	108.93035	13.50	+4231
$^{109}\mathrm{C_9}$	109.00336	09.12	+1103
$^{110}\mathrm{Fe_2}$	109.87155	10.67	-3463
$^{55}\mathrm{Mn_2}$	109.87611	100.00	-4044
$^{94}\mathrm{MoO}$	109.90085	09.02	-45E3
$^{94}\mathrm{ZrO}$	109.90255	17.36	-15E4
$^{110}\mathrm{Cd}$	109.90329	12.39	-----
$^{110}\mathrm{Pd}$	109.90447	11.81	+93E3
$^{110}\mathrm{MoC}$	109.90598	23.62	+41E3
$^{78}\mathrm{SeO_2}$	109.90721	23.42	+28E3
$^{86}\mathrm{SrC_2}$	109.90935	09.64	+18E3
$^{39}\mathrm{K_2O_2}$	109.91724	86.26	+7878
$^{110}\mathrm{Si_3C_2}$	109.92763	08.55	+4515
$^{46}\mathrm{TiO_4}$	109.93227	07.92	+3792
$^{31}\mathrm{P_2O_3}$	109.95226	99.28	+2244
$^{98}\mathrm{RuC}$	109.954/	01.85	+2167
$^{110}\mathrm{C_9}$	110.00670	00.409	+1063
$^{111}\mathrm{Fe_2}$	110.87502	00.26	-3790
$^{95}\mathrm{MoO}$	110.89935	10.73	-23E3
$^{111}\mathrm{Cd}$	110.90428	12.75	-----
$^{99}\mathrm{RuC}$	110.90605	12.58	+63E3
$^{79}\mathrm{BrO_2}$	110.90819	50.29	+28E3
$^{111}\mathrm{SrC_2}$	110.90899	07.09	+24E3
$^{87}\mathrm{RbC_2}$	110.90930	27.24	+22E3
$^{63}\mathrm{CuO_3}$	110.91432	68.59	+11E3
$^{63}\mathrm{CuC_4}$	110.92959	66.08	+4382
$^{47}\mathrm{TiO_4}$	110.93140	06.97	+4089
$^{111}\mathrm{C_9}$	111.01008	00.011	+1048
$^{112}\mathrm{Fe_2}$	111.86388	84.06	-2856
$^{112}\mathrm{Fe_2}$	111.87292	00.04	-3713
$^{96}\mathrm{MoO}$	111.89987	16.49	-35E3
$^{112}\mathrm{Cd}$	111.90306	24.07	-----
$^{96}\mathrm{RuO}$	111.90361	05.50	+20E4
$^{96}\mathrm{ZrO}$	111.90421	02.79	+97E3
$^{112}\mathrm{RuC}$	111.905	12.62	+58E3
$^{112}\mathrm{Sn}$	111.9051	00.96	+55E3
$^{112}\mathrm{SrC_2}$	111.9061	80.89	+37E3
$^{80}\mathrm{SeO_2}$	111.90629	49.36	+35E3
$^{100}\mathrm{MoC}$	111.90651	09.52	+32E3
$^{28}\mathrm{Si_4}$	111.90772	72.30	+24E3
$^{40}\mathrm{Ca_2O_2}$	111.91554	93.58	+8967
$^{48}\mathrm{TiO_4}$	111.92759	73.27	+4562
$^{64}\mathrm{ZnC_4}$	111.92796	46.76	+4494
$^{32}\mathrm{S_2O_3}$	111.92887	89.60	+4336
$^{113}\mathrm{Fe_2}$	112.86735	04.02	-3056
$^{97}\mathrm{MoO}$	112.90112	09.46	-36E3
$^{113}\mathrm{In}$	112.90430	04.28	-----
$^{113}\mathrm{Cd}$	112.90446	12.26	+71E4
$^{113}\mathrm{RuC}$	112.905	17.02	+16E4
$^{89}\mathrm{YC_2}$	112.90572	97.80	+80E3
$^{81}\mathrm{BrO_2}$	112.90622	49.22	+59E3
$^{65}\mathrm{CuO_3}$	112.91251	30.69	+14E3
$^{49}\mathrm{TiO_4}$	112.92751	05.46	+4867
$^{65}\mathrm{CuC_4}$	112.92778	29.56	+4809
$^{27}\mathrm{Al_3O_2}$	112.93444	99.52	+3746
$^{114}\mathrm{Fe_2}$	113.86525	00.66	-2974
$^{57}\mathrm{Fe_2}$	113.87082	00.05	-3481
$^{98}\mathrm{MoO}$	113.90089	23.72	-43E3
$^{114}\mathrm{Cd}$	113.90355	28.86	-----
$^{114}\mathrm{RuC}$	113.90373	31.45	+63E4
$^{114}\mathrm{Sn}$	113.9039	00.66	+33E4
$^{90}\mathrm{ZrC_2}$	113.90433	50.33	+15E4
$^{102}\mathrm{PdC}$	113.90486	00.95	+87E3
$^{82}\mathrm{SeO_2}$	113.90645	09.17	+39E3
$^{50}\mathrm{TiO_4}$	113.92443	05.29	+5455
$^{50}\mathrm{CrO_4}$	113.92569	04.27	+5145
$^{66}\mathrm{ZnC_4}$	113.92605	26.60	+5062
$^{98}\mathrm{RuO}$	113.949/	01.87	+2452
$^{12}\mathrm{C^2_{18}}$	114.00000	80.89	+1181
$^{99}\mathrm{RuO}$	114.90096	12.69	-43E3
$^{115}\mathrm{Sn}$	114.90335	00.35	-44E4
$^{115}\mathrm{In}$	114.90361	95.72	-----
$^{103}\mathrm{RhC}$	114.90455	98.89	+12E4
$^{115}\mathrm{ZrC_2}$	114.90532	12.10	+67E3
$^{90}\mathrm{Zr}^{25}\mathrm{C_2}$	114.90769	01.13	+28E3
$^{58}\mathrm{Ni_2}$	115.87070	47.86	-3681
$^{58}\mathrm{Fe_2}$	115.86662	00.001	-3258
$^{84}\mathrm{SrO_2}$	115.90305	00.56	-14E4
$^{100}\mathrm{RuO}$	115.900	12.59	-53E3
$^{100}\mathrm{MoO}$	115.90142	09.61	-15E4
$^{116}\mathrm{Sn}$	115.90219	14.30	-----
$^{104}\mathrm{PdC}$	115.90328	10.85	+11E4
$^{104}\mathrm{RuC}$	115.90422	18.37	+57E3
$^{116}\mathrm{ZrC_2}$	115.90467	16.98	+47E3
$^{116}\mathrm{Cd}$	115.90499	07.58	+41E3
$^{92}\mathrm{MoC_2}$	115.90855	15.49	+18E3
$^{52}\mathrm{CrO_4}$	115.92015	82.96	+6453
$^{28}\mathrm{Si_3O_2}$	115.92061	78.02	+6298
$^{116}\mathrm{ZnC_4}$	115.92486	17.94	+5113
$^{40}\mathrm{Ca_2C_3}$	115.92517	90.38	+5044
$^{232}\mathrm{Th^2}$	116.0190	100.00	+1185
$^{39}\mathrm{K_3}$	116.89113	80.70	-9766
$^{101}\mathrm{RuO}$	116.9000	17.03	-38E3
$^{85}\mathrm{RbO_2}$	116.90182	71.80	-91E3
$^{117}\mathrm{Sn}$	116.90310	07.61	-----
$^{117}\mathrm{PdC}$	116.90482	22.10	+68E3
$^{93}\mathrm{NbC_2}$	116.90566	97.80	+46E3
$^{85}\mathrm{Si_3O_2}$	116.92017	11.93	+6848
$^{53}\mathrm{CrO_4}$	116.92029	09.46	+6801
$^{27}\mathrm{Al_3C_2}$	116.94462	96.72	+2816
$^{234}\mathrm{U^2}$	117.0202	05.6E3	+ 998
$^{235}\mathrm{U^2}$	117.5214	00.72	
$^{118}\mathrm{Ni_2}$	117.86612	36.29	-3281
$^{59}\mathrm{Co_2}$	117.86636	100.00	-3304
$^{102}\mathrm{RuO}$	117.89864	31.53	-35E3
$^{86}\mathrm{SrO_2}$	117.89915	09.81	-41E3
$^{102}\mathrm{PdO}$	117.89977	00.96	-52E3
$^{118}\mathrm{Sn}$	117.90205	24.03	-----
$^{118}\mathrm{PdC}$	117.90291	27.28	+14E4
$^{106}\mathrm{CdC}$	117.90593	01.20	+30E3
$^{94}\mathrm{MoC_2}$	117.90594	08.84	+30E3
$^{94}\mathrm{ZrC_2}$	117.90764	17.02	+21E3
$^{86}\mathrm{Si_3O_2}$	117.91744	08.45	+7661
$^{54}\mathrm{CrO_4}$	117.91851	02.36	+7163
$^{54}\mathrm{FeO_4}$	117.91925	05.76	+6855
$^{119}\mathrm{Ni_2}$	118.86644	01.65	-3239
$^{119}\mathrm{K_3}$	118.88925	17.89	-8554
$^{87}\mathrm{SrO_2}$	118.89879	06.99	-27E3
$^{87}\mathrm{RbO_2}$	118.89912	27.72	-30E3
$^{103}\mathrm{RhO}$	118.89946	99.76	-32E3
$^{119}\mathrm{Sn}$	118.90315	08.58	-----
$^{119}\mathrm{MoC_2}$	118.90444	10.72	+92E3
$^{107}\mathrm{AgC}$	118.90483	50.78	+71E3
$^{55}\mathrm{MnO_4}$	118.91769	99.04	+8178
$^{238}\mathrm{U^2}$	119.0243	99.274	+ 981
$^{120}\mathrm{Ni_2}$	119.86154	11.94	-2949
$^{40}\mathrm{Ca_3}$	119.88776	90.34	-8303
$^{88}\mathrm{SrO_2}$	119.89592	82.16	-19E3
$^{104}\mathrm{PdO}$	119.89819	10.94	-30E3
$^{104}\mathrm{RuO}$	119.89914	18.53	-39E3
$^{120}\mathrm{Sn}$	119.90220	32.85	-----
$^{108}\mathrm{PdC}$	119.90347	26.41	+94E3
$^{108}\mathrm{CdC}$	119.90407	00.865	+64E3
$^{120}\mathrm{Te}$	119.90449	00.089	+52E3
$^{120}\mathrm{MoC_2}$	119.90496	16.41	+43E3
$^{96}\mathrm{RuC_2}$	119.9087	05.39	+18E3
$^{96}\mathrm{ZrC_2}$	119.90930	02.74	+17E3
$^{56}\mathrm{FeO_4}$	119.91158	90.78	+13E3
$^{27}\mathrm{Al_4C}$	119.92616	98.89	+5004
$^{28}\mathrm{Si_3C_3}$	119.93079	75.83	+4194
$^{12}\mathrm{C_{10}}$	120.00000	89.44	+1226
$^{121}\mathrm{Ni_2}$	120.86186	00.62	-2889
$^{121}\mathrm{K_3}$	120.88737	01.32	-7399
$^{89}\mathrm{YO_2}$	120.89552	99.52	-15E3
$^{105}\mathrm{PdO}$	120.89973	22.18	-30E3
$^{121}\mathrm{Sb}$	120.90371	57.25	-----
$^{109}\mathrm{AgC}$	120.90461	48.11	+13E4
$^{121}\mathrm{MoC_2}$	120.90621	09.61	+48E3
$^{57}\mathrm{FeO_4}$	120.91505	02.17	+11E3
$^{121}\mathrm{Si_3C_3}$	120.93035	14.14	+4538
$^{121}\mathrm{C_{10}}$	121.00335	10.02	+1213
$^{122}\mathrm{Ni_2}$	121.85911	03.41	-2784
$^{110}\mathrm{Fe_2C}$	121.87155	10.55	-3888
$^{55}\mathrm{Mn_2C}$	121.87610	98.89	-4549
$^{122}\mathrm{Ca_3}$	121.88435	01.79	-6572
$^{90}\mathrm{ZrO_2}$	121.89413	51.21	-14E3
$^{106}\mathrm{PdO}$	121.89782	27.26	-24E3
$^{106}\mathrm{CdO}$	121.90084	01.21	-59E3
$^{122}\mathrm{Te}$	121.90290	02.46	-----
$^{110}\mathrm{CdC}$	121.90329	12.25	+31E4
$^{110}\mathrm{PdC}$	121.90447	11.68	+78E3
$^{122}\mathrm{MoC_2}$	121.90598	23.47	+40E3
$^{86}\mathrm{SrC_3}$	121.90935	09.54	+19E3
$^{58}\mathrm{FeO_4}$	121.91295	00.33	+12E3
$^{58}\mathrm{NiO_4}$	121.91499	68.52	+10E3
$^{122}\mathrm{Si_3C_3}$	121.92762	08.60	+4931
$^{98}\mathrm{RuC_2}$	121.954/	01.83	+2386
$^{122}\mathrm{C_{10}}$	122.00670	00.505	+1174
$^{123}\mathrm{Ca_3}$	122.88678	00.41	-7063
$^{91}\mathrm{ZrO_2}$	122.89512	11.17	-14E3
$^{107}\mathrm{AgO}$	122.89974	51.23	-28E3
$^{123}\mathrm{Sb}$	122.90418	42.75	-----
$^{123}\mathrm{CdC}$	122.90428	12.75	+12E5
$^{123}\mathrm{Te}$	122.9043	00.87	+10E5
$^{123}\mathrm{RuC_2}$	122.90605	12.48	+66E3
$^{123}\mathrm{SrC_3}$	122.90899	07.11	+26E3
$^{87}\mathrm{RbC_3}$	122.90930	26.94	+24E3
$^{123}\mathrm{C_{10}}$	123.01008	00.015	+1161
$^{124}\mathrm{Ni_2}$	123.85873	00.57	-2664
$^{56}\mathrm{Fe_2C}$	123.86388	83.09	-3000
$^{124}\mathrm{Ca_3}$	123.88072	05.79	-5053
$^{92}\mathrm{ZrO_2}$	123.89447	17.03	-12E3
$^{92}\mathrm{MoO_2}$	123.89835	15.76	-18E3
$^{108}\mathrm{PdO}$	123.89838	26.55	-18E3
$^{108}\mathrm{CdO}$	123.89898	00.871	-20E3
$^{124}\mathrm{CdC}$	123.90306	23.94	-57E3
$^{124}\mathrm{Te}$	123.90312	04.61	-59E3
$^{124}\mathrm{RuC_2}$	123.905	12.62	-50E4
$^{124}\mathrm{Sn}$	123.90524	05.94	-----
$^{124}\mathrm{SrC_3}$	123.90610	80.08	+14E4
$^{124}\mathrm{Xe}$	123.90612	00.01	+14E4
$^{100}\mathrm{MoC_2}$	123.90651	09.42	+98E3
$^{60}\mathrm{NiO_4}$	123.91041	25.98	+24E3
$^{27}\mathrm{Al_4O}$	123.92107	99.76	+7827
$^{113}\mathrm{Fe_2C}$	124.86735	03.97	-3351
$^{93}\mathrm{NbO_2}$	124.89546	99.52	-14E3
$^{109}\mathrm{AgO}$	124.89952	48.53	-25E3
$^{113}\mathrm{InC}$	124.9043	04.23	-39E4
$^{125}\mathrm{CdC}$	124.90446	12.39	-78E4
$^{125}\mathrm{Te}$	124.90462	06.99	-----
$^{125}\mathrm{RuC_2}$	124.905	16.97	+33E4
$^{63}\mathrm{Cu_2}$	125.85918	47.73	-2817
$^{126}\mathrm{Fe_2C}$	125.86525	00.65	-3260
$^{94}\mathrm{MoO_2}$	125.89574	09.00	-16E3
$^{94}\mathrm{ZrO_2}$	125.89744	17.32	-20E3
$^{110}\mathrm{CdO}$	125.89820	12.36	-22E3
$^{110}\mathrm{PdO}$	125.89938	11.78	-28E3
$^{126}\mathrm{CdC}$	125.90355	28.68	-39E4
$^{126}\mathrm{RuC_2}$	125.90373	31.28	-90E4
$^{126}\mathrm{Te}$	125.90387	18.71	-----

^{126}Te	125.90387	18.71	-----
^{114}SnC	125.90320	00.65	+40E5
^{90}ZrC$_{3}$	125.90433	49.77	+27E4
^{126}Xe	125.90445	00.09	+22E4
^{102}PdC$_{2}$	125.90486	00.94	+13E4
^{252}C$^{2}_{21}$	126.00000	79.14	+1310
^{95}MoO$_{2}$	126.89424	10.71	-12E3
^{111}CdO	126.89919	12.72	-23E3
^{115}SnC	126.90335	00.35	-27E3
^{115}InC	126.90361	94.66	-12E4
^{103}RhC$_{2}$	126.90455	97.80	-72E5
^{127}I	126.90466	100.00	-----
^{127}ZrC$_{3}$	126.90532	12.52	+19E4
^{63}CuO$_{4}$	126.90923	68.43	+28E3
^{254}C$^{2}_{21}$	127.00335	02.085	+1286
^{64}Zn$_{2}$	127.85592	23.91	-2527
^{128}Cu$_{2}$	127.85737	42.71	-2655
^{56}Fe$_{2}$O	127.85879	83.81	-2735
^{128}Ca$_{3}$	127.88053	00.64	-5112
^{52}Cr$_{2}$C$_{2}$	127.88102	68.61	-5214
^{96}MoO$_{2}$	127.89476	16.45	-12E3
^{96}RuO$_{2}$	127.8985	05.48	-13E3
^{112}CdO	127.89797	23.95	-17E3
^{96}ZrO$_{2}$	127.89910	02.79	-20E3
^{112}SnO	127.9000	00.96	-23E3
^{116}SnC	127.90219	14.14	-38E3
^{104}PdC$_{2}$	127.90328	10.73	-56E3
^{128}Xe	127.90351	01.919	-63E3
^{104}RuC$_{2}$	127.90422	18.17	-96E3
^{128}ZrC$_{3}$	127.90467	16.91	-15E4
^{116}CdC	127.90499	07.50	-23E4
^{128}Te	127.90555	31.79	-----
^{40}Ca$_{2}$O$_{3}$	127.90990	92.78	+29E3
^{97}MoO$_{2}$	128.89601	09.41	-15E3
^{113}InO	128.89921	04.27	-23E3
^{113}CdO	128.89937	12.23	-24E3
^{129}SnC	128.9031	07.69	-79E3
^{129}Xe	128.90474	26.44	-----
^{129}PdC$_{2}$	128.90482	21.98	+16E5
^{93}NbC$_{3}$	128.90764	96.72	+45E3
^{27}Al$_{3}$O$_{3}$	128.92935	99.28	+5238
^{130}Zn$_{2}$	129.85401	27.20	-2452
^{65}Cu$_{2}$	129.85556	09.55	-2528
^{98}MoO$_{2}$	129.89578	23.67	-12E3
^{114}CdO	129.89846	28.79	-15E3
^{114}SnO	129.8988	00.66	-16E3
^{130}SnC	129.90205	23.92	-27E3
^{130}PdC$_{2}$	129.90291	27.22	-32E3
^{130}Xe	129.90350	04.08	-37E3
^{106}CdC$_{2}$	129.90593	01.19	-13E4
^{130}Ba	129.90623	00.101	-18E4
^{130}Te	129.90695	34.48	-----
^{94}ZrC$_{3}$	129.90764	16.83	+19E4
^{131}Zn$_{2}$	130.85510	04.02	-2619
^{99}RuO$_{2}$	130.89585	12.66	-14E3
^{115}SnO	130.89826	00.35	-19E3
^{115}InO	130.89852	95.49	-20E3
^{131}SnC	130.90315	08.78	-68E3
^{107}AgC$_{2}$	130.90485	50.22	-52E4
^{131}Xe	130.90508	21.18	-----
^{132}Zn$_{2}$	131.85282	25.89	-2522
^{40}Ca$_{3}$C	131.88776	89.34	-7598
^{100}RuO$_{2}$	131.8948	12.56	-13E3
^{100}MoO$_{2}$	131.89631	09.58	-15E3
^{116}SnO	131.89710	14.27	-16E3
^{116}CdO	131.89990	07.54	-25E3
^{132}SnC	131.90220	32.58	-45E3
^{108}PdC$_{2}$	131.90347	26.12	-80E3
^{108}CdC$_{2}$	131.90407	00.86	-13E4
^{132}Xe	131.90416	26.89	-14E4
^{120}TeC	131.90449	00.087	-21E4
^{132}Ba	131.90512	00.097	-----
^{28}Si$_{3}$O$_{3}$	131.91552	77.83	+13E3
^{27}Al$_{4}$C$_{2}$	131.92616	97.80	+6269
^{12}C$_{11}$	132.00000	88.45	+1390
^{133}Zn$_{2}$	132.85318	02.29	-2558
^{101}RuO$_{2}$	132.8948	16.99	-13E3
^{85}RbO$_{3}$	132.8968	71.63	-16E3
^{117}SnO	132.89801	07.59	-19E3
^{133}Cs	132.90513	100.00	-----
^{109}AgC$_{2}$	132.90461	47.58	+26E4
^{85}RbC$_{4}$	132.91202	69.01	+19E3
^{85}Si$_{3}$O$_{3}$	132.91508	11.90	+13E3
^{133}C$_{11}$	133.00335	10.90	+1353
^{134}Zn$_{2}$	133.85091	10.50	-2510
^{67}Zn$_{2}$	133.85423	00.17	-2680
^{110}Fe$_{2}$C$_{2}$	133.87155	10.43	-4094
^{55}Mn$_{2}$C$_{2}$	133.87610	97.80	-4757
^{102}RuO$_{2}$	133.89353	31.46	-13E3
^{86}SrO$_{3}$	133.89410	09.79	-13E3
^{118}SnO	133.89696	23.97	-18E3
^{122}TeC	133.9029	02.43	-99E3
^{110}CdC$_{2}$	133.90329	12.12	-14E4
^{122}SnC	133.90346	04.67	-17E4
^{134}Ba	133.90425	02.42	-----
^{110}PdC$_{2}$	133.90447	11.55	+61E4
^{86}SrC$_{4}$	133.90935	09.43	+26E3
^{86}Si$_{3}$O$_{3}$	133.91235	08.43	+17E3
^{134}C$_{11}$	134.00670	00.611	+1307
^{135}Zn$_{2}$	134.85200	01.53	-2519
^{87}SrO$_{3}$	134.89372	06.97	-11E3
^{87}RbO$_{3}$	134.89403	27.65	-12E3
^{103}RhO$_{2}$	134.89435	99.52	-12E3
^{119}SnO	134.89806	08.56	-18E3
^{123}SbC	134.90418	42.28	-98E3
^{135}CdC$_{2}$	134.90428	12.86	-11E4
^{135}Ba	134.90555	06.59	-----
^{27}Al^{5}	134.90770	100.00	+63E3
^{68}Zn$_{2}$	135.84972	03.45	-2487
^{112}Fe$_{2}$C$_{2}$	135.86388	82.20	-3356
^{40}Ca$_{3}$O	135.88267	90.12	-6263
^{88}SrO$_{3}$	135.89083	81.96	-10E3
^{104}PdO$_{2}$	135.89308	10.92	-12E3
^{104}RuO$_{2}$	135.89402	18.49	-13E3
^{120}SnO	135.89711	32.77	-19E3
^{120}TeO	135.89940	00.089	-27E3
^{124}TeC	135.89898	04.56	-25E3
^{136}CdC$_{2}$	135.90306	23.82	-10E4
^{136}Ba	135.90437	07.81	-----
^{112}SnC$_{2}$	135.9051	00.94	+19E4
^{124}SnC	135.90524	05.87	+16E4
^{136}SrC$_{4}$	135.90610	79.26	+79E3
^{136}Ce	135.90707	00.193	+50E3
^{136}Xe	135.90721	08.87	+48E3
^{137}Fe$_{2}$C$_{2}$	136.86735	05.77	-3582
^{89}YO$_{3}$	136.89042	99.28	-9037
^{105}PdO$_{2}$	136.89462	22.12	-13E3
^{121}SbO	136.89862	57.11	-20E3
^{113}InC$_{2}$	136.90430	04.19	-11E4
^{137}CdC$_{2}$	136.90446	12.52	-12E4
^{137}TeC	136.90462	06.96	-14E4
^{137}Ba	136.90557	11.32	-----
^{69}Ga$_{2}$	137.85142	36.48	-2580
^{90}ZrO$_{3}$	137.88906	51.09	-8717
^{106}PdO$_{2}$	137.89271	27.20	-12E3
^{106}CdO$_{2}$	137.89573	01.21	-15E3
^{122}TeO	137.89781	02.45	-20E3
^{122}SnO	137.89837	04.71	-21E3
^{138}CdC$_{2}$	137.90355	28.49	-10E4
^{138}TeC	137.90387	18.58	-14E4
^{114}SnC$_{2}$	137.9039	00.65	-14E4
^{90}ZrC$_{4}$	137.90433	49.22	-25E4
^{138}Ba	137.90488	71.66	-----
^{138}Ce	137.90603	00.25	+12E4
^{138}La	137.90674	00.089	+74E3
^{91}ZrO$_{3}$	138.89002	11.14	-8676
^{107}AgO$_{2}$	138.89463	51.10	-12E3
^{123}SbO	138.89909	42.65	-20E3
^{123}TeO	138.8992	00.87	-20E3
^{139}SnC$_{2}$	138.90335	00.35	-52E3
^{115}InC$_{2}$	138.90361	93.61	-57E3
^{127}IC	138.90466	98.89	-10E4
^{139}ZrC$_{4}$	138.90532	12.94	-20E4
^{139}La	138.90603	99.911	-----
^{139}BaH	138.91270	71.65	+20E3
^{70}Ge$_{2}$	139.84798	04.21	-2442
^{140}Ga$_{2}$	139.85053	47.84	-2555
^{140}Ti$_{3}$	139.85321	01.42	-2687
^{28}Si$_{5}$	139.88465	66.66	-6733
^{92}ZrO$_{3}$	139.88940	16.99	-8810
^{108}PdO$_{2}$	139.89327	26.58	-12E3
^{124}TeO	139.89803	04.58	-19E3
^{124}SnO	139.90015	05.93	-27E3
^{116}SnC$_{2}$	139.90219	13.99	-45E3
^{140}ZrC$_{4}$	139.90467	16.84	-23E4
^{116}CdC$_{2}$	139.90499	07.41	-48E4
^{140}Ce	139.90528	88.48	-----
^{128}TeC	139.90555	31.44	+52E4
^{139}LaH	139.91385	99.90	+16E3
^{27}Al$_{4}$O$_{2}$	[illegible]	[illegible]	+13E3
^{141}Ti$_{3}$	140.85234	02.63	-2555
^{93}NbO$_{3}$	140.89039	99.28	-8250
^{109}AgO$_{2}$	140.89441	48.42	-11E3
^{125}TeO	140.89953	06.96	-18E3
^{141}SnC$_{2}$	140.9031	07.75	-32E3
^{128}TeC	140.90555	31.44	-73E3
^{93}NbC$_{4}$	140.90566	95.65	-77E3
^{141}Pr	140.90743	100.00	-----
^{140}CeH	140.91310	88.47	+25E3
^{142}Ge$_{2}$	141.84558	11.23	-2227
^{142}Ti$_{3}$	141.84853	14.51	-2335
^{71}Ga$_{2}$	141.84964	15.68	-2379
^{110}Fe$_{2}$O$_{2}$	141.86137	10.62	-2961
^{55}Mn$_{2}$O$_{2}$	141.86592	99.52	-3271
^{107}AgCl	141.87368	38.78	-3984
^{94}ZrO$_{3}$	141.89237	17.27	-8382
^{110}CdO$_{2}$	141.89309	12.33	-8754
^{110}PdO$_{2}$	141.89427	11.75	-9442
^{126}TeO	141.89878	18.66	-14E3
^{142}SnC$_{2}$	141.90205	23.67	-20E3
^{130}BaC	141.90623	00.100	-46E3
^{130}TeC	141.90695	34.10	-60E3
^{142}Nd	141.90748	27.11	-78E3
^{94}ZrC$_{4}$	141.90764	16.64	-86E3
^{142}Ce	141.90930	11.07	-----
^{127}IO	142.89957	99.76	-14E3
^{143}SnC$_{2}$	142.90315	08.92	-22E3
^{143}Nd	142.90958	12.17	-----
^{142}NdH	142.91530	27.11	+25E3
^{142}CeH	142.91712	11.07	+19E3
^{72}Ge$_{2}$	143.84318	07.52	-2160
^{144}Ti$_{3}$	143.84385	44.17	-2182
^{144}Ge$_{2}$	143.84499	22.51	-2220
^{56}Fe$_{2}$O$_{2}$	143.85370	83.61	-2565
^{109}AgCl	143.87346	12.57	-3683
^{40}Ca$_{3}$C$_{2}$	143.88776	88.35	-6529
^{112}CdO$_{2}$	143.89286	23.95	-8495
^{128}TeO	143.90046	31.70	-15E3
^{144}SnC$_{2}$	143.9022	32.32	-19E3
^{132}BaC	143.90512	00.096	-31E3
^{144}Nd	143.90980	23.85	-----
^{144}Sm	143.91165	03.09	+78E3
^{27}Al$_{4}$C$_{3}$	143.92616	96.72	+8800
^{12}C$_{12}$	144.00000	87.46	+1595
^{145}Ti$_{3}$	144.84377	10.78	-2122
^{145}Ge$_{2}$	144.84493	04.15	-2159
^{113}InO$_{2}$	144.89410	04.26	-8069
^{113}CdO$_{2}$	144.89426	12.20	-8141
^{121}SbC$_{2}$	144.90371	55.99	-17E3
^{133}CsC	144.90513	98.89	-21E3
^{145}Nd	144.91206	08.30	-----
^{145}C$_{12}$	145.00335	11.78	+1587
^{146}Ti$_{3}$	145.84069	09.64	-2027
^{146}Ge$_{2}$	145.84259	23.83	-2081
^{109}AgCl	145.87051	11.90	-3459
^{114}CdO$_{2}$	145.89335	28.72	-7545
^{130}BaC	145.90114	00.101	-13E3
^{130}TeO	145.90186	34.30	-14E3
^{122}TeC$_{2}$	145.9029	02.41	-15E3
^{122}SnC$_{2}$	145.90346	04.62	-16E3
^{134}BaC	145.90425	02.39	-17E3
^{146}Nd	145.91269	17.22	-----
^{146}C$_{12}$	146.00670	00.725	+1552
^{147}Ti$_{3}$	146.84061	01.39	-1989
^{147}Ge$_{2}$	146.84434	05.67	-2094
^{115}InO$_{2}$	146.89341	95.26	-6969
^{123}SbC$_{2}$	146.90418	41.81	-14E3
^{147}BaC	146.90555	06.55	-16E3
^{134}Ba^{13}C	46.90760	00.026	-21E3
^{27}Al$_{5}$C	146.90770	98.39	-22E3
^{147}Sm	146.91449	14.97	-----
^{147}C$_{12}$	147.01003	00.027	+1537
^{148}Ti$_{3}$	147.83752	00.68	-1874
^{148}Ge$_{2}$	147.84200	17.61	-1987
^{56}Fe$_{2}$C$_{3}$	147.86388	81.26	-2313
^{116}SnO$_{2}$	147.89199	14.23	-6045
^{116}CdO$_{2}$	147.89479	07.54	-6826
^{124}TeC$_{2}$	147.89898	00.189	-8462
^{132}BaO	147.90003	00.097	-9000
^{148}BaC	147.90437	07.79	-12E3
^{135}Ba^{13}C	47.90891	00.07	-20E3
^{124}SnC$_{2}$	147.90524	05.81	-13E3
^{136}CeC	147.90707	00.191	-16E3
^{148}Sm	147.91442	11.24	-73E3
^{148}Nd	147.91646	05.73	-----

$^{149}\text{Ge}_2$	148.84463	01.20	-2063
$^{85}\text{RbO}_4$	148.89170	71.46	-5933
$^{117}\text{SnO}_2$	148.89290	07.57	-6230
^{133}CsO	148.90004	99.76	-8885
$^{149}\text{TeC}_2$	148.90462	06.94	-12E3
^{149}BaC	148.90557	11.28	-13E3
^{149}BaC	148.90772	00.086	-16E3
^{149}Sm	148.91680	13.83	-----
$^{150}\text{Ge}_2$	149.84229	05.67	-1909
$^{75}\text{As}_2$	149.84342	100.00	-1937
$^{86}\text{SrO}_4$	149.88899	09.77	-4712
^{134}BaO	149.89916	02.35	-6921
$^{150}\text{TeC}_2$	149.90387	18.45	-8845
^{150}BaC	149.90488	71.00	-9405
^{138}CeC	149.90603	00.25	-10E3
^{138}LaC	149.90674	00.088	-11E3
^{150}Sm	149.91690	07.44	-38E3
^{150}Nd	149.92082	05.62	-----
$^{87}\text{SrO}_4$	150.88863	06.95	-4883
$^{87}\text{RbO}_4$	150.88894	27.58	-4932
$^{119}\text{SnO}_2$	150.89295	08.54	-5676
^{135}BaO	150.90046	06.57	-7909
$^{27}\text{Al}_5\text{O}$	150.90261	99.76	-8914
$^{127}\text{IC}_2$	150.90466	97.80	-10E3
^{151}BaC	150.90824	00.79	-13E3
^{151}Eu	150.91954	47.82	-----
$^{152}\text{Cr}_3$	151.83261	00.47	-1751
$^{152}\text{Se}_2$	151.83856	01.22	-1880
$^{40}\text{Ca}_3\text{O}_2$	151.87758	89.91	-3636
$^{88}\text{SrO}_4$	151.88574	81.77	-4519
$^{120}\text{SnO}_2$	151.89200	32.69	-5553
^{136}BaO	151.89928	07.79	-7566
^{140}CeC	151.90528	87.50	-11E3
$^{128}\text{TeC}_2$	151.90555	31.09	-11E3
^{152}LaC	151.90938	01.106	-15E3
^{152}Sm	151.91936	26.72	-----
^{152}Gd	151.91943	00.20	+20E5
$^{153}\text{Se}_2$	152.83926	01.37	-1880
$^{89}\text{YO}_4$	152.88536	99.04	-4339
$^{121}\text{SbO}_2$	152.89351	56.97	-5645
^{137}BaO	152.90048	11.29	-7600
^{141}PrC	152.90748	98.89	-12E3
^{153}CeC	152.90863	00.979	-13E3
^{153}Eu	152.9206	52.18	-----
$^{154}\text{Cr}_3$	153.82707	09.07	-1623
$^{156}\text{Se}_2$	153.83667	05.68	-1805
$^{90}\text{ZrO}_4$	153.88397	50.97	-4055
$^{122}\text{TeO}_2$	153.8927	02.45	-5266
$^{122}\text{SnO}_2$	153.8933	04.70	-5376
^{138}BaO	153.89979	71.49	-6952
^{138}LaO	153.90165	00.089	-7590
^{138}CeO	153.90094	00.25	-7333
$^{130}\text{BaC}_2$	153.90623	00.099	-9804
$^{130}\text{TeC}_2$	153.90695	33.72	-10E3
^{142}NdC	153.90748	26.81	-11E3
^{142}CeC	153.9093	10.95	-12E3
^{154}Gd	153.92094	02.15	-16E4
^{154}Sm	153.92193	22.71	-----
$^{155}\text{Cr}_3$	154.82721	02.07	-1622
$^{155}\text{Se}_2$	154.83737	03.56	-1816
$^{91}\text{ZrO}_4$	154.88496	11.11	-4105
$^{123}\text{SbO}_2$	154.89398	42.54	-5394
^{139}LaO	154.90094	99.67	-7120
^{155}NdC	154.90958	12.30	-12E3
^{155}CeC	154.91265	00.123	-15E3
^{155}Gd	154.9227	14.73	-----
$^{156}\text{Cr}_3$	155.82153	59.40	-1548
$^{156}\text{Se}_2$	155.83575	14.68	-1802
$^{92}\text{ZrO}_4$	155.88431	16.95	-4108
$^{40}\text{Ca}_3\text{C}_3$	155.88776	87.37	-4519
$^{124}\text{TeO}_2$	155.88878	04.59	-4657
$^{124}\text{SnO}_2$	155.89504	05.91	-5728
$^{132}\text{BaC}_2$	155.90512	00.095	-9097
^{156}NdC	155.9098	23.72	-13E3
^{144}SmC	155.91165	03.06	-15E3
^{156}Gd	155.92226	20.47	-----
$^{156}\text{C}_{13}$	156.00000	86.49	+2006
$^{157}\text{Cr}_3$	156.82167	20.10	-1532
$^{157}\text{Se}_2$	156.83645	07.55	-1790
$^{93}\text{NbO}_4$	156.88530	99.04	-4044
$^{125}\text{TeO}_2$	156.89442	06.96	-5287
$^{133}\text{CsC}_2$	156.90513	97.80	-8272
^{141}PrO	156.90239	99.76	-7228
^{145}NdC	156.91206	08.47	-15E3
^{157}Gd	156.9241	15.68	-----
$^{157}\text{C}_{13}$	157.00335	12.60	+1980
$^{158}\text{Cr}_3$	157.81989	07.31	-1511
$^{158}\text{Se}_2$	157.83386	02.29	-1744
$^{79}\text{Br}_2$	157.83678	25.54	-1802
$^{94}\text{ZrO}_4$	157.88728	17.23	-4257
$^{126}\text{TeO}_2$	157.89367	18.62	-5139
^{142}NdO	157.90239	27.04	-7175
^{142}CeO	157.90421	11.04	-7822
$^{134}\text{BaC}_2$	157.90425	02.37	-7837
^{158}NdC	157.91269	17.12	-14E3
^{158}Dy	157.92401	00.09	-41E4
^{158}Gd	157.9244	24.87	-----
$^{158}\text{C}_{13}$	158.00335	00.847	+2000
$^{159}\text{Cr}_3$	158.82003	01.23	-1516
$^{159}\text{Se}_2$	158.83661	01.39	-1800
^{143}NdO	158.90449	12.14	-7794
$^{159}\text{BaC}_2$	158.90555	06.50	-8221
^{147}SmC	158.91449	14.80	-15E3
^{159}Tb	158.92488	100.00	-----
$^{159}\text{C}_{13}$	159.01008	00.038	+1865
$^{160}\text{Se}_2$	159.83294	29.14	-1696
$^{160}\text{Br}_2$	159.83481	49.99	-1731
$^{56}\text{Fe}_2\text{O}_3$	159.84861	83.41	-2035
$^{128}\text{TeO}_2$	159.8535	31.64	-2170
$^{160}\text{BaC}_2$	159.90437	07.78	-7000
^{144}NdO	159.90477	23.79	-7127
^{144}SmO	159.90656	03.08	-7745
$^{136}\text{CeC}_2$	159.90707	00.189	-7941
^{160}SmC	159.91442	11. 29	-13E3
^{148}NdC	159.91646	05.67	-15E3
^{160}Dy	159.9239	02.294	-48E3
^{160}Gd	159.92721	21.90	-----
$^{161}\text{BaC}_2$	160.90557	11.36	-7994
^{145}NdO	160.90697	08.28	-8592
^{161}SmC	160.9168	13.80	-18E3
^{161}Dy	160.9257	18.88	-----
$^{81}\text{Br}_2$	161.83284	24.47	-1746
$^{162}\text{Se}_2$	161.83310	09.15	-1751
$^{130}\text{BaO}_2$	161.89603	00.101	-5476
$^{130}\text{TeO}_2$	161.89675	34.31	-5613
$^{27}\text{Al}_6$	161.88924	100.00	-4453
$^{162}\text{BaC}_2$	161.90488	70.33	-7815
$^{138}\text{CeC}_2$	161.90603	00.245	-8274
^{162}SmC	161.9169	07.51	-19E3
^{150}NdC	161.92082	05.56	-34E3
^{162}Dy	161.9256	25.53	-----
^{162}Er	161.92873	00.136	+52E3
$^{163}\text{BaC}_2$	162.90824	01.57	-8330
$^{139}\text{LaC}_2$	162.90603	99.71	-7884
^{147}SmO	162.90940	14.93	-8855
^{151}EuC	162.91954	47.29	-20E3
^{163}Dy	162.9278	24.97	-----
$^{164}\text{Fe}_3$	163.81415	00.93	-1434
$^{164}\text{Se}_2$	163.83326	00.84	-1721
$^{132}\text{BaO}_2$	163.89492	00.097	-4882
$^{140}\text{CeC}_2$	163.90528	86.53	-7060
^{148}SmO	163.90933	11.21	-8551
^{148}NdO	163.91138	05.72	-9575
^{152}SmC	163.91936	26.42	-18E3
^{152}GdC	163.91943	00.198	-18E3
^{164}Dy	163.9285	28.18	-----
^{164}Er	163.9298	01.56	+13E3
$^{55}\text{Mn}_3$	164.81415	100.00	-1435
$^{133}\text{CsO}_2$	164.89493	99.52	-4827
$^{141}\text{PrC}_2$	164.90748	97.80	-7629
^{149}SmO	164.91171	13.80	-9484
^{153}EuC	164.9206	51.60	-19E3
$^{165}\text{CeC}_2$	164.90864	01.94	-8061
^{165}Ho	164.9291	100.00	-----
$^{166}\text{Fe}_3$	165.80349	14.67	-1325
$^{134}\text{BaO}_2$	165.89405	02.41	-4789
$^{142}\text{NdC}_2$	165.90748	26.51	-7819
$^{142}\text{CeC}_2$	165.90930	10.83	-8553
^{150}SmO	165.91181	07.42	-9824
^{150}NdO	165.91573	05.61	-13E3
^{154}GdC	165.92094	02.13	-21E3
^{154}SmC	165.92193	22.46	-44E3
^{166}Er	165.9287	33.41	-----
$^{167}\text{Fe}_2$	166.80995	00.70	-1385
$^{135}\text{BaO}_2$	166.89535	06.56	-4749
$^{167}\text{NdC}_2$	166.90958	12.49	-7979
$^{167}\text{CeC}_2$	166.91265	00.242	-9352
^{151}EuO	166.91445	47.70	-10E3
^{167}GdC	166.9227	14.59	-21E3
^{167}Er	166.9305	22.94	-----
$^{168}\text{Fe}_3$	167.79582	77.12	-1244
$^{28}\text{Si}_7$	167.86158	56.68	-2426
$^{40}\text{Ca}_3\text{O}_3$	167.87249	89.69	-2880
$^{136}\text{BaO}_2$	167.89417	07.77	-4585
$^{136}\text{CeO}_2$	167.89687	00.192	-4949
$^{168}\text{NdC}_2$	[illegible]	[illegible]	-7996
$^{144}\text{SmC}_2$	167.91165	03.02	-8769
^{156}DyC	167.914	00.052	-9996
^{152}SmO	167.91427	26.66	-10E3
^{152}GdO	167.91434	00.20	-10E3
^{168}GdC	167.92226	20.40	-21E3
^{168}Er	167.9308	27.07	-----
^{168}Yb	167.93390	00.135	+54E3
$^{12}\text{C}_{14}$	168.00000	85.53	+2427
$^{169}\text{Fe}_3$	168.79929	05.52	-1251
$^{137}\text{BaO}_2$	168.89537	11.27	-4335
$^{169}\text{NdC}_2$	168.91206	08.64	-7582
^{153}EuO	168.91551	52.05	-8972
^{169}GdC	168.9241	15.74	-17E3
^{169}Tm	168.93434	100.00	-----
$^{169}\text{C}_{14}$	169.00335	13.42	+2448
$^{170}\text{Fe}_3$	169.80319	00.96	-1283
$^{170}\text{Sr}_2$	169.82260	00.11	-1504
$^{85}\text{Rb}_2$	169.82404	52.06	-1523
$^{138}\text{BaO}_2$	169.89468	71.32	-4153
$^{138}\text{CeO}_2$	169.89585	00.25	-4275
$^{138}\text{LaO}_2$	169.89654	00.089	-4351
$^{134}\text{BaC}_3$	169.90425	02.34	-5421
$^{146}\text{NdC}_2$	169.91269	16.84	-7418
^{154}GdO	169.91585	02.14	-8604
^{154}SmO	169.91684	22.66	-9058
^{158}DyC	169.924	00.089	-15E3
^{170}GdC	169.9244	24.76	-15E3
^{170}Yb	169.934/	03.03	-11E4
^{170}Er	169.9356	14.88	-----
$^{170}\text{C}_{14}$	170.00670	00.977	+2390
$^{171}\text{Sr}_2$	170.82224	00.079	-1503
$^{139}\text{LaO}_2$	170.89583	97.43	-4255
$^{171}\text{BaC}_3$	170.90555	06.45	-5614
$^{147}\text{SmC}_2$	170.91449	14.64	-7947
^{155}GdO	170.91761	14.69	-9295
^{159}TbC	170.92488	98.89	-15E3
^{171}Yb	170.936/	14.31	-----
$^{171}\text{C}_{14}$	171.01008	00.044	+2307
$^{172}\text{Sr}_2$	171.81935	01.90	-1624
$^{172}\text{Rb}_2$	171.82132	40.19	-1655
$^{140}\text{CeO}_2$	171.89508	88.05	-5708
^{160}DyC	171.9239	02.27	-13E4
$^{172}\text{BaC}_3$	171.90437	07.76	-8254
^{156}DyO	171.909	00.052	-11E3
$^{172}\text{SmC}_2$	171.91442	11.31	-16E3
$^{148}\text{NdC}_2$	171.91646	05.60	-20E3
^{156}GdO	171.91717	20.42	-21E3
^{160}GdC	171.92721	21.66	-86E3
^{172}Yb	171.9252/	21.82	-----
$^{173}\text{Sr}_2$	172.81834	01.38	-1445
$^{141}\text{PrO}_2$	172.89728	99.52	-4247
$^{173}\text{BaC}_3$	172.90557	11.20	-5333
$^{173}\text{SmC}_2$	172.9168	13.78	-8157
^{157}GdO	172.91901	15.64	-9107
^{173}DyC	172.9257	18.70	-14E3
^{173}Yb	172.938/	16.13	-----
$^{58}\text{Ni}_3$	173.80605	33.11	-1455
$^{174}\text{Sr}_2$	173.81545	16.77	-1579
$^{174}\text{Rb}_2$	173.81860	07.76	-1625
$^{142}\text{NdO}_2$	173.89728	26.98	-6141
$^{142}\text{CeO}_2$	173.8991	11.02	-6563
$^{174}\text{BaC}_3$	173.90488	69.68	-8394
$^{174}\text{SmC}_2$	173.9169	07.58	-20E3
^{158}DyO	173.919	00.09	-26E3
^{158}GdO	173.91931	24.81	-28E3
$^{150}\text{NdC}_2$	173.92082	05.50	-36E3
^{174}DyC	173.9256	25.46	INF.
^{174}Yb	173.9256	31.84	-----
^{162}ErC	173.92873	00.134	+56E3
^{174}Hf	173.939	00.18	+13E3
$^{175}\text{Sr}_2$	174.81509	11.59	-1378
$^{143}\text{NdO}_2$	174.89938	12.11	-4105
$^{139}\text{LaC}_3$	174.90603	96.63	-4864
$^{151}\text{EuC}_2$	174.91954	46.77	-7789
^{159}TbO	174.91979	99.76	-7877
^{175}DyC	174.9278	24.97	-12E3
^{175}Lu	174.942/	97.41	-----
$^{176}\text{Ni}_3$	175.80147	37.66	-1246
$^{176}\text{Sr}_2$	175.81202	68.16	-1346
$^{144}\text{NdO}_2$	175.8996	23.74	-4080
$^{144}\text{SmO}_2$	175.90145	03.08	-4263
$^{140}\text{CeC}_3$	175.90528	85.57	-4699
^{160}DyO	175.91881	02.29	-7359
$^{152}\text{SmC}_2$	175.91936	26.13	-7532
$^{152}\text{GdC}_2$	175.91943	00.20	-7554
^{160}GdO	175.92212	21.85	-8541
^{176}DyC	175.9285	28.15	-12E3
^{164}ErC	175.9298	01.54	-14E3

$^{176}\mathrm{Hf}$	175.92212	05.20	-8541
$^{176}\mathrm{Lu}$	175.9419	02.59	-22E3
$^{176}\mathrm{Yb}$	175.94272	12.73	-----
$^{59}\mathrm{Co}_3$	176.79954	100.00	-1238
$^{177}\mathrm{Ni}_3$	176.80179	01.71	-1257
$^{145}\mathrm{NdO}_2$	176.90186	08.26	-4354
$^{153}\mathrm{EuC}_2$	176.9206	51.03	-8080
$^{161}\mathrm{DyO}$	176.92061	18.83	-8083
$^{165}\mathrm{HoC}$	176.9291	98.89	-13E3
$^{177}\mathrm{Hf}$	176.9425	18.50	-----
$^{178}\mathrm{Ni}_3$	177.79689	19.53	-1218
$^{89}\mathrm{Y}_2$	177.81144	100.00	-1353
$^{146}\mathrm{NdO}_2$	177.90249	17.14	-4393
$^{162}\mathrm{DyO}$	177.92051	25.47	-7912
$^{154}\mathrm{GdC}_2$	177.92094	02.10	-8066
$^{154}\mathrm{SmC}_2$	177.92193	22.21	-8445
$^{162}\mathrm{ErO}$	177.92364	00.136	-9191
$^{166}\mathrm{ErC}$	177.9287	33.04	-12E3
$^{178}\mathrm{Hf}$	177.9430	27.14	-----
$^{179}\mathrm{Ni}_3$	178.79720	01.30	-1209
$^{147}\mathrm{SmO}_2$	178.90429	14.90	-4374
$^{179}\mathrm{GdC}_2$	178.9227	14.73	-7953
$^{163}\mathrm{DyO}$	178.92271	24.86	-7957
$^{179}\mathrm{ErC}$	178.9305	23.05	-12E3
$^{179}\mathrm{Hf}$	178.9452	13.75	-----
$^{180}\mathrm{Ni}_3$	179.79446	07.37	-1187
$^{90}\mathrm{Zr}_2$	179.80866	26.48	-1309
$^{148}\mathrm{SmO}_2$	179.90422	26.48	-4297
$^{148}\mathrm{NdO}_2$	179.9065	05.70	-4544
$^{180}\mathrm{GdC}_2$	179.92226	20.34	-7548
$^{164}\mathrm{DyO}$	179.92341	28.11	-7931
$^{164}\mathrm{ErO}$	179.92471	01.56	-8413
$^{180}\mathrm{ErC}$	179.9308	27.02	-12E3
$^{168}\mathrm{YbC}$	179.9339	00.134	-15E3
$^{180}\mathrm{W}$	179.9445	00.135	-11E4
$^{180}\mathrm{Ta}$	179.945/	00.012	-16E4
$^{180}\mathrm{Hf}$	179.9461	35.24	-----
$^{12}\mathrm{C}_{15}$	180.00000	84.58	+3339
$^{181}\mathrm{Ni}_3$	180.79262	00.43	-1181
$^{181}\mathrm{Zr}_2$	180.80965	11.56	-1329
$^{149}\mathrm{SmO}_2$	180.9066	13.76	-4616
$^{165}\mathrm{HoO}$	180.9241	99.76	-8339
$^{181}\mathrm{GdC}_2$	180.9241	15.78	-8339
$^{169}\mathrm{TmC}$	180.9343	98.89	-16E3
$^{181}\mathrm{Ta}$	180.9458	98.988	-----
$^{181}\mathrm{C}_{15}$	181.00335	14.22	+3144
$^{182}\mathrm{Ni}_3$	181.78987	02.22	-1165
$^{182}\mathrm{Zr}_2$	181.80900	18.87	-1328
$^{134}\mathrm{BaO}_3$	181.88898	02.40	-3191
$^{134}\mathrm{BaC}_4$	181.90425	02.31	-4358
$^{150}\mathrm{SmO}_2$	181.90670	07.40	-4630
$^{150}\mathrm{NdO}_2$	181.91062	05.59	-5143
$^{166}\mathrm{ErO}$	181.92361	33.33	-8126
$^{182}\mathrm{GdC}_2$	181.924	24.66	-8270
$^{170}\mathrm{YbC}$	181.934/	03.00	-15E3
$^{170}\mathrm{ErC}$	181.9356	14.72	-18E3
$^{182}\mathrm{W}$	181.9460	26.41	-----
$^{182}\mathrm{C}_{15}$	182.00670	1.115	+2997
$^{183}\mathrm{Zr}_2$	182.80999	03.84	-1325
$^{183}\mathrm{Ni}_3$	182.79019	00.12	-1159
$^{135}\mathrm{BaO}_3$	182.89028	06.54	-3164
$^{183}\mathrm{BaC}_4$	182.90555	06.40	-4300
$^{159}\mathrm{TbC}_2$	182.92488	97.80	-7879
$^{167}\mathrm{ErO}$	182.92541	22.88	-8063
$^{183}\mathrm{YbC}$	182.9360	14.18	-15E3
$^{183}\mathrm{W}$	182.9481	14.40	-----
$^{183}\mathrm{C}_{15}$	183.01008	00.054	+2952
$^{184}\mathrm{Ni}_3$	183.78744	00.49	-1139
$^{184}\mathrm{Zr}_2$	183.80934	20.83	-1318
$^{184}\mathrm{Mo}_2$	183.81710	02.51	-1396
$^{136}\mathrm{BaO}_3$	183.88910	07.75	-3076
$^{184}\mathrm{BaC}_4$	183.90437	07.73	-4131
$^{160}\mathrm{DyC}_2$	183.9239	02.24	-7358
$^{152}\mathrm{SmO}_2$	183.90916	26.59	-4629
$^{184}\mathrm{YbC}$	183.9252	21.74	-7762
$^{168}\mathrm{ErO}$	183.9257	27.00	-7932
$^{160}\mathrm{GdC}_2$	183.92721	21.41	-8481
$^{168}\mathrm{YbO}$	183.9288	00.135	-9156
$^{184}\mathrm{Os}$	183.946	00.018	-63E3
$^{184}\mathrm{W}$	183.9489	30.64	-----
$^{185}\mathrm{Ni}_3$	184.78776	00.03	-1154
$^{185}\mathrm{Zr}_2$	184.81296	03.91	-1370
$^{137}\mathrm{BaO}_3$	184.89030	11.24	-3205

$^{153}\mathrm{EuO}_2$	184.9140	51.93	-4919
$^{185}\mathrm{BaC}_4$	184.90557	11.17	-4359
$^{185}\mathrm{DyC}_2$	184.9257	18.52	-8294
$^{169}\mathrm{TmO}$	184.9292	99.76	-9843
$^{185}\mathrm{YbC}$	184.938	16.37	-19E3
$^{185}\mathrm{Re}$	184.948	37.07	-----
$^{186}\mathrm{Ni}_3$	185.78501	00.09	-1122
$^{93}\mathrm{Nb}_2$	185.81132	100.00	-1334
$^{186}\mathrm{Zr}_2$	185.81231	08.83	-1344
$^{186}\mathrm{Mo}_2$	185.81449	02.86	-1365
$^{138}\mathrm{BaO}_3$	185.88961	71.14	-3044
$^{186}\mathrm{BaC}_4$	185.90488	70.03	-4058
$^{154}\mathrm{GdO}_2$	185.91074	02.14	-4653
$^{154}\mathrm{SmO}_2$	185.91173	22.60	-4772
$^{186}\mathrm{YbC}$	185.9256	31.67	-7408
$^{186}\mathrm{DyC}_2$	185.9256	25.38	-7408
$^{162}\mathrm{ErC}_2$	185.92873	00.133	-8464
$^{170}\mathrm{YbO}$	185.9290	03.02	-8569
$^{170}\mathrm{ErO}$	185.9356	14.84	-12E3
$^{174}\mathrm{HfC}$	185.939	00.18	-16E3
$^{186}\mathrm{W}$	185.9507	28.41	-----
$^{186}\mathrm{Os}$	185.952	01.59	+14E4
$^{187}\mathrm{Ni}_3$	186.78738	00.003	-1129
$^{187}\mathrm{Mo}_2$	186.81299	04.98	-1335
$^{187}\mathrm{Zr}_2$	186.81462	00.63	-1351
$^{139}\mathrm{LaO}_3$	186.89076	99.19	-3004
$^{155}\mathrm{GdO}_2$	186.9125	14.66	-4516
$^{187}\mathrm{DyC}_2$	186.9278	24.98	-7419
$^{171}\mathrm{YbO}$	186.9310	14.28	-8498
$^{175}\mathrm{LuC}$	186.942	96.33	-17E3
$^{187}\mathrm{Re}$	186.953/	62.93	-----
$^{187}\mathrm{Os}$	186.956/	01.64	+62E3
$^{188}\mathrm{Ni}_3$	187.78463	00.014	-1091
$^{188}\mathrm{Zr}_2$	187.81528	03.99	-1327
$^{188}\mathrm{Mo}_2$	187.81188	06.05	-1311
$^{140}\mathrm{CeO}_3$	187.89001	87.84	-2810
$^{140}\mathrm{CeC}_4$	187.90528	84.63	-3641
$^{156}\mathrm{GdO}_2$	187.91206	20.37	-4192
$^{172}\mathrm{YbO}$	187.9201	21.76	-5108
$^{188}\mathrm{DyC}_2$	187.9285	28.11	-6618
$^{164}\mathrm{ErC}_2$	187.9298	01.53	-6936
$^{176}\mathrm{HfC}$	187.9408	05.14	-12E3
$^{188}\mathrm{LuC}$	187.9419	03.64	-13E3
$^{176}\mathrm{YbC}$	187.94272	12.59	-13E3
$^{188}\mathrm{Os}$	187.9569	02.59	-----
$^{63}\mathrm{Cu}_3$	188.78877	32.98	-1113
$^{189}\mathrm{Mo}_2$	188.81476	05.84	-1315
$^{27}\mathrm{Al}_7$	188.87078	100.00	-2154
$^{157}\mathrm{GdO}_2$	188.91390	15.60	-4237
$^{165}\mathrm{HoC}_2$	188.9291	97.80	-6427
$^{173}\mathrm{YbO}$	188.9330	16.09	-7410
$^{189}\mathrm{HfC}$	188.9425	18.36	-12E3
$^{189}\mathrm{Os}$	188.9585	16.1	-----
$^{190}\mathrm{Ni}_3$	189.78425	00.001	-1057
$^{190}\mathrm{Mo}_2$	189.81453	12.99	-1271
$^{190}\mathrm{Zr}_2$	189.81694	00.97	-1291
$^{158}\mathrm{GdO}_2$	189.9142	24.75	-3815
$^{174}\mathrm{YbO}$	189.9205	31.76	-4367
$^{166}\mathrm{ErC}_2$	189.9287	32.67	-5381
$^{174}\mathrm{HfO}$	189.9339	00.18	-6311
$^{190}\mathrm{HfC}$	189.9430	27.04	-9046
$^{190}\mathrm{Pt}$	189.964	00.013	-----
$^{191}\mathrm{Cu}_3$	190.78696	44.26	-1082
$^{191}\mathrm{Mo}_2$	190.80940	06.91	-1240
$^{159}\mathrm{TbO}_2$	190.91468	99.52	-3920
$^{191}\mathrm{ErC}_2$	190.9305	23.16	-5804
$^{175}\mathrm{LuO}$	190.9369	97.18	-7206
$^{191}\mathrm{HfC}$	190.9452	13.90	-11E3
$^{191}\mathrm{Ir}$	190.9634	37.3	-----
$^{64}\mathrm{Zn}_3$	191.78388	11.69	-1077
$^{192}\mathrm{Mo}_2$	191.81192	13.05	-1277
$^{96}\mathrm{Zr}_2$	191.81860	00.078	-1337
$^{192}\mathrm{Ru}_2$	191.81740	00.31	-1326
$^{160}\mathrm{DyO}_2$	191.9137	02.28	-3958
$^{160}\mathrm{GdO}_2$	191.91703	21.80	-4250
$^{192}\mathrm{ErC}_2$	191.9308	26.97	-6113
$^{168}\mathrm{YbC}_2$	191.9339	00.132	-6783
$^{176}\mathrm{HfO}$	191.9357	05.19	-7244
$^{176}\mathrm{LuO}$	191.9368	02.58	-7558
$^{176}\mathrm{YbO}$	191.9376	12.70	-7803
$^{180}\mathrm{WC}$	191.9445	00.134	-11E3
$^{180}\mathrm{TaC}$	191.945	00.012	-11E3
$^{192}\mathrm{HfC}$	191.9461	35.00	-12E3
$^{192}\mathrm{Os}$	191.9622	41.0	-----
$^{192}\mathrm{Pt}$	191.9648	00.78	+74E3
$^{12}\mathrm{C}_{16}$	192.00000	83.64	+5078

$^{193}\mathrm{Cu}_3$	192.78515	19.80	-1063
$^{193}\mathrm{Mo}_2$	192.81042	10.60	-1235
$^{161}\mathrm{DyO}_2$	192.9155	18.79	-3769
$^{169}\mathrm{TmC}_2$	192.9343	97.80	-5956
$^{177}\mathrm{HfO}$	192.9374	18.46	-6586
$^{181}\mathrm{TaC}$	192.9458	98.88	-9233
$^{193}\mathrm{Ir}$	192.9667/	62.7	-----
$^{193}\mathrm{C}_{16}$	193.00335	14.99	+5265
$^{194}\mathrm{Zn}_3$	193.78197	19.95	-1070
$^{194}\mathrm{Mo}_2$	193.81094	10.49	-1273
$^{194}\mathrm{Ru}_2$	193.86270	00.21	-1928
$^{162}\mathrm{DyO}_2$	193.9154	25.41	-4049
$^{170}\mathrm{YbC}_2$	193.934	02.96	-6620
$^{170}\mathrm{ErC}_2$	193.9356	14.55	-7002
$^{178}\mathrm{HfO}$	193.9379	27.07	-7636
$^{182}\mathrm{WC}$	193.9460	26.12	-11E3
$^{194}\mathrm{Pt}$	193.9633/	32.9	-----
$^{194}\mathrm{C}_{16}$	194.00670	01.26	+4469
$^{195}\mathrm{Zn}_3$	194.78306	02.95	-1065
$^{195}\mathrm{Mo}_2$	194.81219	07.53	-1266
$^{195}\mathrm{Ru}_2$	194.81475	01.40	-1287
$^{163}\mathrm{DyO}_2$	194.91760	24.85	-4012
$^{195}\mathrm{YbC}_2$	194.9360	14.06	-6456
$^{179}\mathrm{HfO}$	194.9401	13.72	-7470
$^{195}\mathrm{WC}$	194.9481	14.53	-11E3
$^{195}\mathrm{Pt}$	194.9662/	33.8	-----
$^{195}\mathrm{C}_{16}$	195.01008	00.066	+4443
$^{196}\mathrm{Zn}_3$	195.78078	24.65	-1052
$^{196}\mathrm{Mo}_2$	195.81196	08.84	-1263
$^{196}\mathrm{Ru}_2$	195.81370	01.43	-1277
$^{28}\mathrm{Si}_7$	195.83851	56.68	-1524
$^{164}\mathrm{ErO}_2$	195.91960	01.55	-4126
$^{164}\mathrm{DyO}_2$	195.92340	23.04	-4484
$^{196}\mathrm{YbC}_2$	195.9252	21.65	-4677
$^{180}\mathrm{WO}$	195.9394	00.135	-7075
$^{180}\mathrm{HfO}$	195.9410	35.16	-7508
$^{180}\mathrm{TaO}$	195.9399	00.012	-7205
$^{184}\mathrm{OsC}$	195.946/	00.018	-9288
$^{196}\mathrm{WC}$	195.9489	30.46	-11E3
$^{196}\mathrm{Hg}$	195.96583	00.146	-15E4
$^{196}\mathrm{Pt}$	195.9671/	25.3	-----
$^{197}\mathrm{Zn}_3$	196.78115	03.35	-1059
$^{197}\mathrm{Mo}_2$	196.81272	01.82	-1275
$^{197}\mathrm{Ru}_2$	196.81370	02.36	-1283
$^{197}\mathrm{Si}_7$	196.83806	20.22	-1525
$^{165}\mathrm{HoO}_2$	196.9189	99.52	-4078
$^{197}\mathrm{YbC}_2$	196.938/	16.24	-6745
$^{181}\mathrm{TaO}$	196.9407	99.747	-7432
$^{185}\mathrm{ReC}$	196.948/	36.66	-10E3
$^{197}\mathrm{Au}$	196.9672	100.00	-----
$^{198}\mathrm{Zn}_3$	197.77814	17.99	-1062
$^{198}\mathrm{Ru}_2$	197.81243	05.57	-1298
$^{198}\mathrm{Mo}_2$	197.81249	04.58	-1301
$^{198}\mathrm{Si}_7$	197.83533	16.39	-1531
$^{134}\mathrm{BaO}_4$	197.88390	02.40	-2453
$^{166}\mathrm{ErO}_2$	197.9185	33.25	-4294
$^{198}\mathrm{YbC}_2$	197.9256	31.14	-5076
$^{174}\mathrm{HfC}_2$	197.939/	00.75	-7733
$^{182}\mathrm{WO}$	197.9409	26.65	-8353
$^{186}\mathrm{WC}$	197.9507	28.10	-14E3
$^{188}\mathrm{OsC}$	197.952/	01.57	-16E3
$^{198}\mathrm{Pt}$	197.9646	07.21	-----
$^{198}\mathrm{Hg}$	197.96675	10.02	+92E3
$^{199}\mathrm{Zn}_3$	198.77996	03.19	-1057
$^{199}\mathrm{Ru}_2$	198.8111	03.34	-1266
$^{199}\mathrm{Si}_7$	198.83489	04.33	-1492
$^{135}\mathrm{BaO}_4$	198.88519	06.53	-2397
$^{167}\mathrm{ErO}_2$	198.9203	22.83	-4152
$^{175}\mathrm{LuC}_2$	198.942/	95.27	-7588
$^{183}\mathrm{WO}$	198.9430	14.33	-7889
$^{187}\mathrm{ReC}$	198.953/	62.23	-13E3
$^{187}\mathrm{OsC}$	198.956/	01.62	-16E3
$^{199}\mathrm{Hg}$	198.96822	16.84	-----
$^{200}\mathrm{Zn}_3$	199.77696	10.01	-1045
$^{200}\mathrm{Ru}_2$	199.81110	09.16	-1263
$^{200}\mathrm{Mo}_2$	199.81302	00.93	-1288
$^{200}\mathrm{Si}_7$	199.83216	01.87	-1469
$^{136}\mathrm{BaO}_4$	199.88401	07.73	-2371
$^{168}\mathrm{ErO}_2$	199.92060	26.94	-4190
$^{176}\mathrm{HfC}_2$	199.9408	05.09	-7264
$^{200}\mathrm{LuC}_2$	199.9419	04.66	-7317
$^{176}\mathrm{YbC}_2$	199.94272	12.45	-7308
$^{184}\mathrm{OsO}$	199.9409	00.018	-7290
$^{184}\mathrm{WO}$	199.9438	30.57	-8152
$^{188}\mathrm{OsC}$	199.9569	13.2	-13E3
$^{200}\mathrm{Hg}$	199.96833	22.13	-----

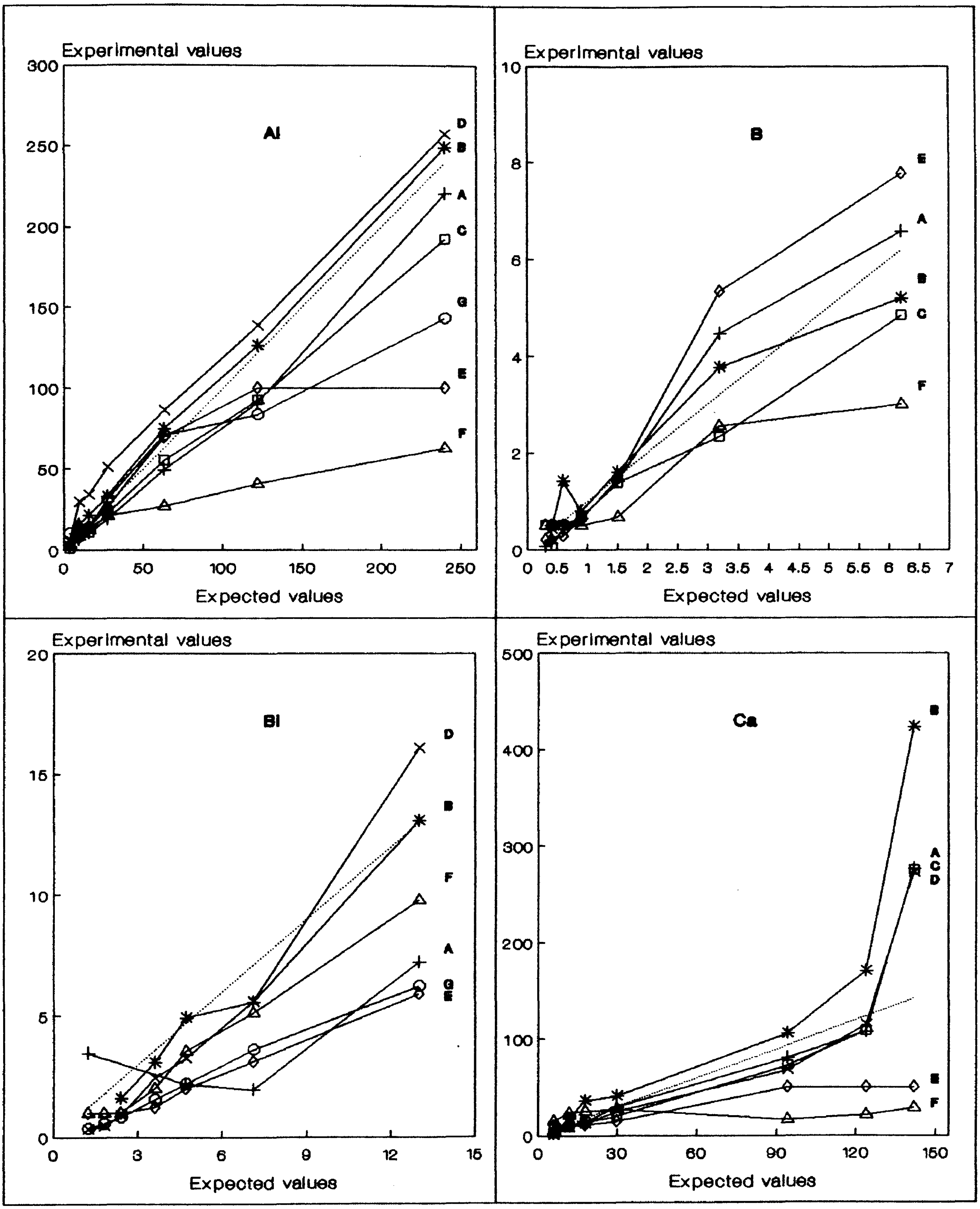
$^{201}\mathrm{Zn}_3$	200.77805	01.36	-1045
$^{201}\mathrm{Ru}_2$	200.80978	12.35	-1252
$^{137}\mathrm{BaO}_4$	200.88521	11.21	-2362
$^{169}\mathrm{TmO}_2$	200.9241	99.52	-4351
$^{201}\mathrm{HfC}_2$	200.9425	18.20	-7232
$^{185}\mathrm{ReO}$	200.943/	36.98	-7364
$^{201}\mathrm{OsC}$	200.9585	16.0	-17E3
$^{201}\mathrm{Hg}$	200.97209	13.22	-----
$^{202}\mathrm{Zn}_3$	201.77577	03.45	-1037
$^{202}\mathrm{Ru}_2$	201.8087	11.58	-1247
$^{138}\mathrm{BaO}_4$	201.88452	70.97	-2346
$^{170}\mathrm{YbO}_2$	201.9238	03.03	-4313
$^{170}\mathrm{ErO}_2$	201.9254	14.81	-4467
$^{202}\mathrm{HfC}_2$	201.9430	26.95	-7311
$^{186}\mathrm{WO}$	201.9456	28.35	-8071
$^{202}\mathrm{OsC}$	201.9548	26.3	-13E3
$^{202}\mathrm{Hg}$	201.97063	29.80	-----
$^{203}\mathrm{Zn}_3$	202.77685	00.47	-1041
$^{203}\mathrm{Ru}_2$	202.8087/	15.52	-1244
$^{171}\mathrm{YbO}_2$	202.9258	14.24	-4403
$^{203}\mathrm{HfC}_2$	202.9452	14.04	-7602
$^{187}\mathrm{ReO}$	202.948/	62.78	-8493
$^{187}\mathrm{OsO}$	202.9510	01.64	-9712
$^{191}\mathrm{IrC}$	202.9634	37.3	-24E3
$^{203}\mathrm{Tl}$	202.9719	29.50	-----
$^{204}\mathrm{Zn}_3$	203.77451	00.84	-1027
$^{204}\mathrm{Ru}_2$	203.80746	14.68	-1232
$^{140}\mathrm{CeO}_4$	203.88492	87.63	-2314
$^{172}\mathrm{YbO}_2$	203.9150	21.71	-3512
$^{180}\mathrm{WC}_2$	203.9445	00.132	-7137
$^{180}\mathrm{TaC}_2$	203.9458	00.012	-7477
$^{204}\mathrm{HfC}_2$	203.9461	34.76	-7560
$^{192}\mathrm{OsC}$	203.9622	40.55	-19E3
$^{192}\mathrm{PtC}$	203.9648	00.77	-25E3
$^{204}\mathrm{Pb}$	203.97308	01.48	-----
$^{204}\mathrm{Hg}$	203.97347	06.85	+52E4
$^{12}\mathrm{C}_{17}$	204.00000	82.72	+7577
$^{205}\mathrm{Zn}_3$	204.77505	00.067	-1031
$^{205}\mathrm{Ru}_2$	204.8092	06.34	-1245
$^{173}\mathrm{YbO}_2$	204.9278	16.05	-4456
$^{181}\mathrm{TaC}_2$	204.9458	97.79	-7320
$^{189}\mathrm{OsO}$	204.9534	16.1	-10E3
$^{193}\mathrm{IrC}$	204.9667	62.0	-29E3
$^{205}\mathrm{Tl}$	204.9738	70.50	-----
$^{205}\mathrm{C}_{17}$	205.00335	15.75	+6937
$^{206}\mathrm{Zn}_3$	205.77505	00.067	-1033
$^{206}\mathrm{Ru}_2$	205.80795	11.75	-1237
$^{206}\mathrm{Pd}_2$	205.80814	00.21	-1239
$^{206}\mathrm{Rh}_2$	205.80910	100.00	-1246
$^{174}\mathrm{YbO}_2$	205.9154	31.69	-3489
$^{182}\mathrm{WC}_2$	205.9460	25.83	-7242
$^{190}\mathrm{OsO}$	205.9497	26.3	-8326
$^{194}\mathrm{PtC}$	205.9633	32.5	-18E3
$^{206}\mathrm{Pb}$	205.97444	26.4	-----
$^{206}\mathrm{C}_{17}$	206.00670	01.41	+6385
$^{207}\mathrm{Pd}_2$	206.80968	00.43	-1245
$^{175}\mathrm{LuO}_2$	206.9318	96.94	-4695
$^{207}\mathrm{WC}_2$	206.9481	14.66	-7451
$^{191}\mathrm{IrO}$	206.9583	37.2	-12E3
$^{207}\mathrm{PtC}$	206.9662	33.8	-21E3
$^{207}\mathrm{Pb}$	206.97588	22.6	-----
$^{207}\mathrm{C}_{17}$	207.01008	00.079	+6052
$^{208}\mathrm{Zn}_3$	207.77554	00.002	-1034
$^{208}\mathrm{Pd}_2$	207.80656	01.73	-1223
$^{208}\mathrm{Ru}_2$	207.80844	03.45	-1236
$^{176}\mathrm{HfO}_2$	207.9306	05.17	-4516
$^{176}\mathrm{LuO}_2$	207.9317	02.58	-4627
$^{176}\mathrm{YbO}_2$	207.9325	12.67	-4711
$^{208}\mathrm{WC}_2$	207.9489	30.29	-7495
$^{192}\mathrm{OsO}$	207.9571	40.9	-11E3
$^{192}\mathrm{PtO}$	207.9579	00.78	-13E3
$^{208}\mathrm{PtC}$	207.9671	25.37	-22E3
$^{208}\mathrm{Pb}$	207.97665	52.3	-----
$^{209}\mathrm{Pd}_2$	208.80810	04.88	-1220
$^{177}\mathrm{HfO}_2$	208.9323	18.41	-4443
$^{185}\mathrm{ReC}_2$	208.948	36.25	-6668
$^{193}\mathrm{IrO}$	208.9616	62.5	-12E3
$^{197}\mathrm{AuC}$	208.9672	98.89	-17E3
$^{209}\mathrm{Bi}$	208.97934	100.00	-----
$^{210}\mathrm{Pd}_2$	209.80619	11.45	-1381
$^{178}\mathrm{HfO}_2$	209.80964	27.01	-8266
$^{186}\mathrm{WC}_2$	209.9507	27.78	-28E3
$^{186}\mathrm{OsC}_2$	209.952	01.55	-34E3
$^{194}\mathrm{PtO}$	209.9582	32.8	-----
$^{198}\mathrm{PtC}$	209.9646	07.13	+33E3
$^{211}\mathrm{HgC}$	209.96675	16.76	+25E3
$^{211}\mathrm{Pd}_2$	210.80773	12.15	-1376
$^{187}\mathrm{ReC}_2$	210.953	61.54	-27E3
$^{195}\mathrm{PtO}$	210.9611	33.7	-----
$^{199}\mathrm{HgC}$	210.96822	16.65	+30E3
$^{212}\mathrm{Pd}_2$	211.80582	13.55	-1357
$^{180}\mathrm{HfO}_2$	211.9359	35.07	-8121
$^{196}\mathrm{PtO}$	211.9620	25.2	-----
$^{212}\mathrm{HgC}$	211.96833	23.06	+34E3
$^{213}\mathrm{Pd}_2$	212.80829	11.88	-1385
$^{181}\mathrm{TaO}_2$	212.9356	99.51	-8036
$^{197}\mathrm{AuO}$	212.9621	99.76	-----
$^{213}\mathrm{HgC}$	212.97029	13.33	+26E3
$^{214}\mathrm{Pd}_2$	213.80638	17.19	-1378
$^{214}\mathrm{Ag}_2$	213.80966	26.37	-1408
$^{187}\mathrm{WO}_2$	213.9358	26.28	-8274
$^{198}\mathrm{PtO}$	213.9595	02.19	-99E3
$^{198}\mathrm{HgO}$	213.96166	10.00	-----
$^{214}\mathrm{HgC}$	213.97063	29.62	+24E3
$^{215}\mathrm{Pd}_2$	214.80695	05.25	-1397
$^{183}\mathrm{WO}_2$	214.9379	14.33	-8520
$^{199}\mathrm{HgO}$	214.96313	16.80	-----
$^{203}\mathrm{TlC}$	214.9719	29.17	+25E3
$^{216}\mathrm{Pd}_2$	215.80694	13.58	-1119
$^{216}\mathrm{Ag}_2$	215.80944	49.96	-1134
$^{184}\mathrm{WO}_2$	215.9387	30.49	-3524
$^{200}\mathrm{HgO}$	215.96323	23.07	-5874
$^{204}\mathrm{PbC}$	215.97308	01.46	-8024
$^{204}\mathrm{HgC}$	215.97347	06.77	-8142
$^{12}\mathrm{C}_{18}$	216.00000	81.80	-----
$^{217}\mathrm{Cd}_2$	216.81021	00.31	-1124
$^{186}\mathrm{WO}_2$	216.9405	28.27	-5688
$^{205}\mathrm{TlC}$	216.9738	69.72	-7344
$^{217}\mathrm{C}_{18}$	217.00335	16.50	-----
$^{218}\mathrm{Cd}_2$	217.80736	00.80	-1094
$^{218}\mathrm{Pd}_2$	217.80794	06.31	-1097
$^{218}\mathrm{Ag}_2$	217.80922	23.67	-1104
$^{202}\mathrm{HgO}$	217.96553	29.73	-5295
$^{206}\mathrm{PbC}$	217.97444	23.3	-6758
$^{218}\mathrm{C}_{18}$	218.00670	01.571	-----
$^{219}\mathrm{Cd}_2$	218.80835	00.52	-1086
$^{203}\mathrm{TlO}$	218.9668	29.43	-5060
$^{219}\mathrm{PbC}$	218.97588	22.7	-6404
$^{219}\mathrm{C}_{18}$	219.01008	00.094	-----
$^{220}\mathrm{Cd}_2$	219.80658	02.66	-1363
$^{220}\mathrm{Pd}_2$	219.80894	01.39	-1383
$^{204}\mathrm{PbO}$	219.96799	01.48	-----
$^{204}\mathrm{HgO}$	219.96838	06.83	+57E4
$^{220}\mathrm{PbC}$	219.97665	52.0	+25E3
$^{221}\mathrm{Cd}_2$	220.80757	03.37	-1371
$^{205}\mathrm{TlO}$	220.9687	70.3	-----
$^{209}\mathrm{BiC}$	220.97934	98.89	+21E3
$^{222}\mathrm{Cd}_2$	221.80635	08.28	-1362
$^{206}\mathrm{PbO}$	221.96935	23.5	-----
$^{223}\mathrm{Cd}_2$	222.80734	08.27	-1364
$^{207}\mathrm{PbO}$	222.97080	22.5	-----
$^{224}\mathrm{Cd}_2$	223.80684	16.20	-1360
$^{224}\mathrm{Si}_8$	223.81544	52.27	-1435
$^{208}\mathrm{PbO}$	223.97156	52.1	-----
$^{75}\mathrm{As}_3$	224.76513	100.00	-1076
$^{225}\mathrm{Cd}_2$	224.80783	13.26	-1352
$^{209}\mathrm{BiO}$	224.97425	99.76	-----
$^{226}\mathrm{Cd}_2$	225.80661	17.27	
$^{227}\mathrm{Cd}_2$	226.80801	09.01	
$^{228}\mathrm{Cd}_2$	227.80710	11.98	-1182
$^{228}\mathrm{In}_2$	227.80791	08.19	-1188
$^{204}\mathrm{PbC}_2$	227.97308	01.45	-8470
$^{228}\mathrm{C}_{19}$	228.00000	80.89	-----
$^{229}\mathrm{Cd}_2$	228.80945	01.86	-1181
$^{229}\mathrm{C}_{19}$	229.00335	17.22	-----
$^{230}\mathrm{In}_2$	229.80722	91.62	-1153
$^{230}\mathrm{Cd}_2$	229.80854	04.38	-1161
$^{230}\mathrm{C}_{19}$	230.00670	01.74	-----
$^{231}\mathrm{PbC}_2$	230.97588	22.6	
$^{232}\mathrm{Sn}_2$	231.80638	03.05	-1002
$^{232}\mathrm{Cd}_2$	231.80998	00.57	-1018
$^{232}\mathrm{PbC}_2$	231.97665	51.6	-3782
$^{232}\mathrm{Th}$	232.0380	100.00	-----
$^{233}\mathrm{Sn}_2$	232.80529	02.46	-----
$^{209}\mathrm{BiC}_2$	232.97934	97.80	+1338
$^{234}\mathrm{Sn}_2$	233.80424	08.04	- 991
$^{234}\mathrm{U}$	234.0403	00.0056	----
$^{235}\mathrm{Sn}_2$	234.80515	06.34	- 989
$^{235}\mathrm{U}$	235.0428	00.7204	----
$^{236}\mathrm{Sn}_2$	235.80439	16.65	
$^{237}\mathrm{Sn}_2$	236.80530	09.16	-1497
$^{205}\mathrm{TlO}_2$	236.9636	70.20	-----
$^{238}\mathrm{Sn}_2$	237.80425	17.95	- 974
$^{206}\mathrm{PbO}_2$	237.96424	23.5	-2822
$^{238}\mathrm{U}$	238.0486	99.2739	----
$^{239}\mathrm{Sn}_2$	238.80535	06.40	-1490
$^{207}\mathrm{PbO}_2$	238.96568	22.5	-----
$^{240}\mathrm{Sn}_2$	239.80440	14.76	-1227
$^{208}\mathrm{PbO}_2$	239.96645	52.0	-7154
$^{240}\mathrm{C}_{20}$	240.00000	79.99	-----
$^{241}\mathrm{Sn}_2$	240.80661	01.71	-1225
$^{241}\mathrm{C}_{20}$	241.00335	17.93	-----
$^{242}\mathrm{Sn}_2$	241.80566	05.96	-1204
$^{242}\mathrm{C}_{20}$	242.00670	01.91	-----
$^{243}\mathrm{Sn}_2$	242.80839	01.02	-1205
$^{243}\mathrm{C}_{20}$	243.01008	00.128	-----
$^{244}\mathrm{Sn}_2$	243.80692	04.13	
$^{232}\mathrm{ThC}$	244.0380	98.89	
$^{232}\mathrm{ThO}$	248.0329	99.76	
$^{238}\mathrm{UC}$	250.0486	98.175	
$^{252}\mathrm{C}_{21}$	252.00000	79.14	
$^{253}\mathrm{C}_{21}$	253.00335	18.62	
$^{254}\mathrm{C}_{21}$	254.00670	02.09	-----
$^{238}\mathrm{UO}$	254.0435	99.035	+5930
$^{232}\mathrm{ThC}_2$	256.0380	97.80	
$^{238}\mathrm{UC}_2$	262.0486	97.088	
$^{232}\mathrm{ThO}_2$	264.0278	99.52	9496
$^{264}\mathrm{C}_{22}$	264.00000	78.26	-----
$^{265}\mathrm{C}_{22}$	265.00335	19.29	
$^{266}\mathrm{C}_{22}$	266.00670	02.27	
$^{238}\mathrm{UO}_2$	270.0384	98.796	

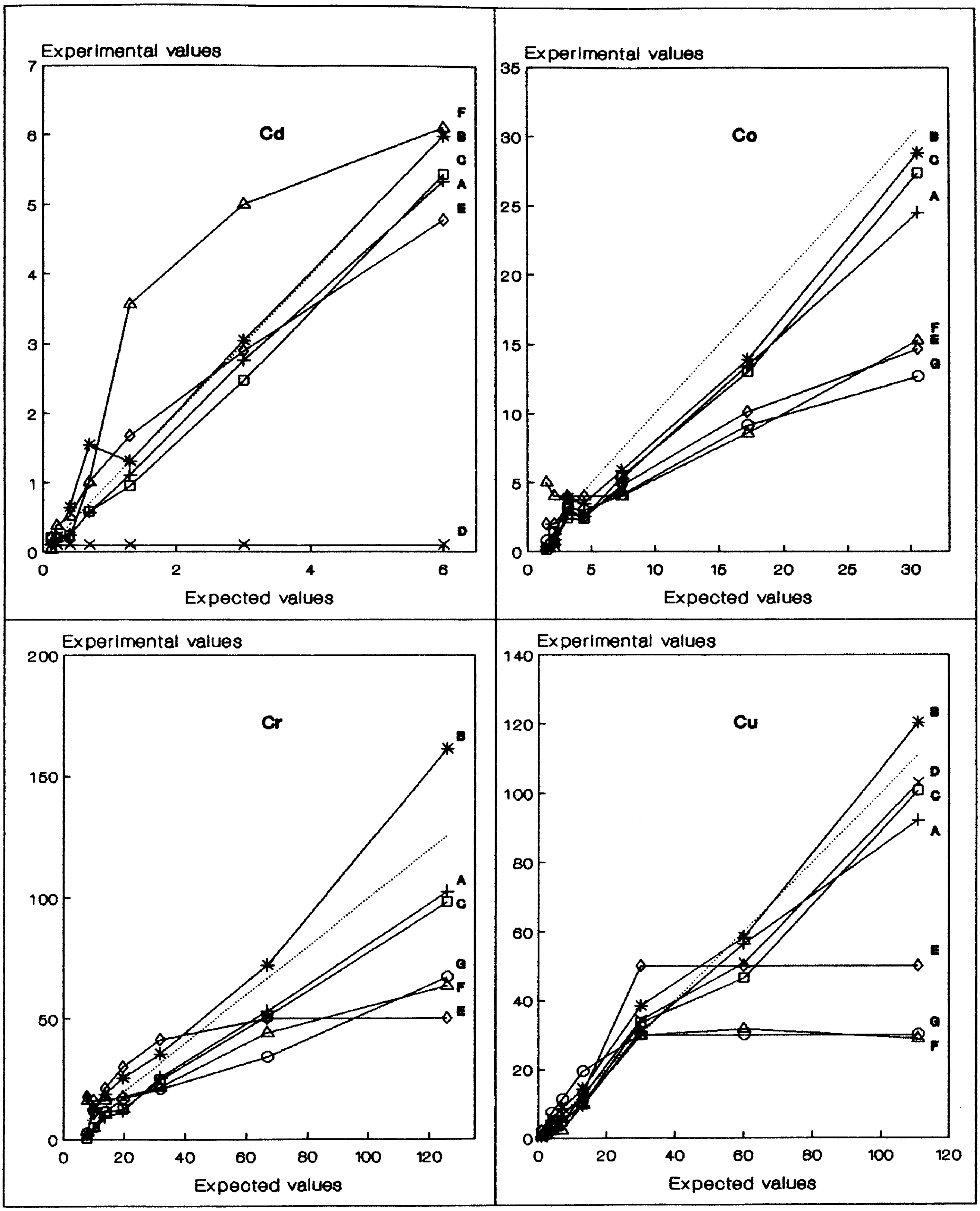
APPENDIX C

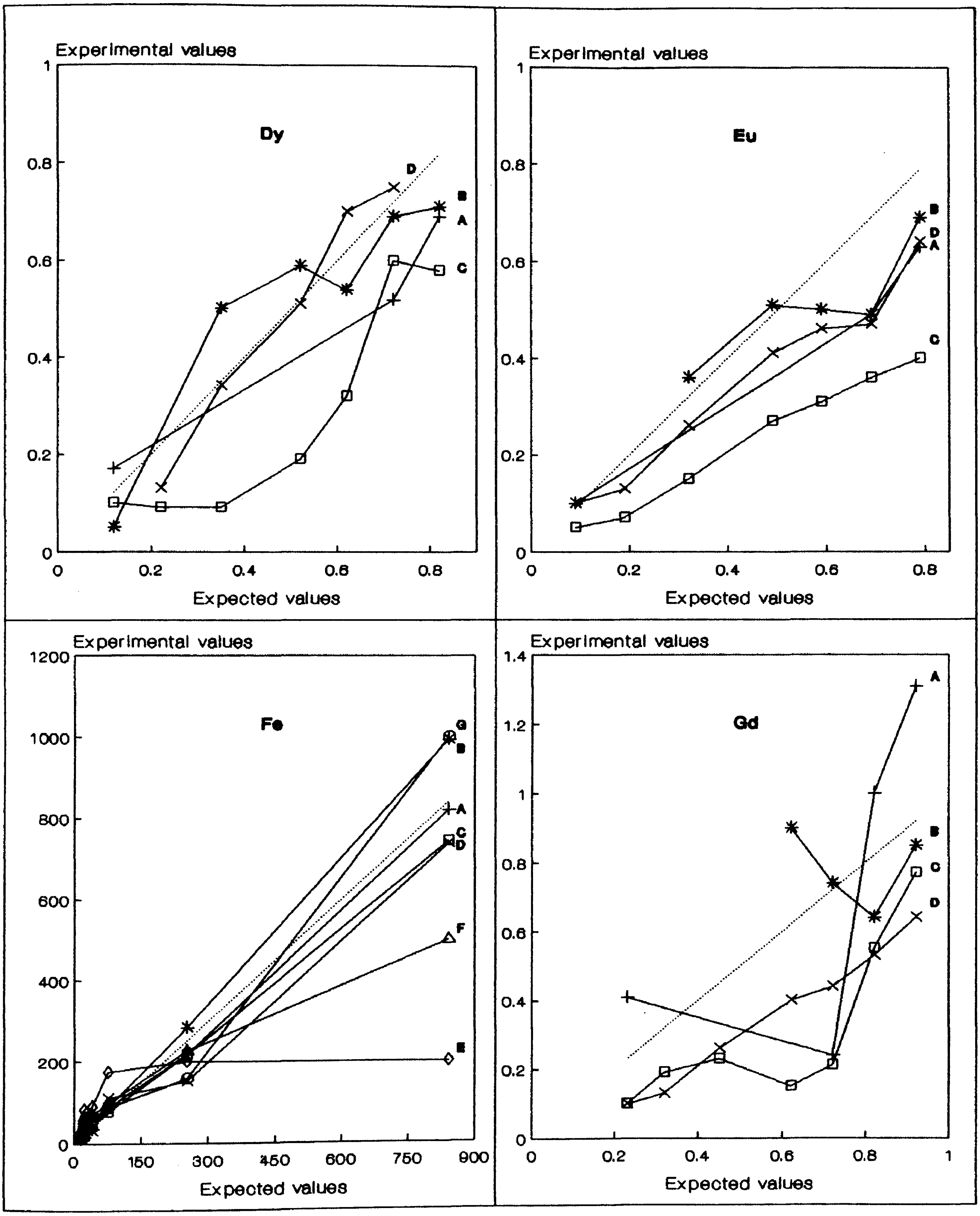
COMPARISON OF EXPERIMENTAL ANALYTICAL DATA TO EXPECTED VALUES FOR SELECTED ELEMENTS USING VARIOUS ANALYTICAL TECHNIQUES

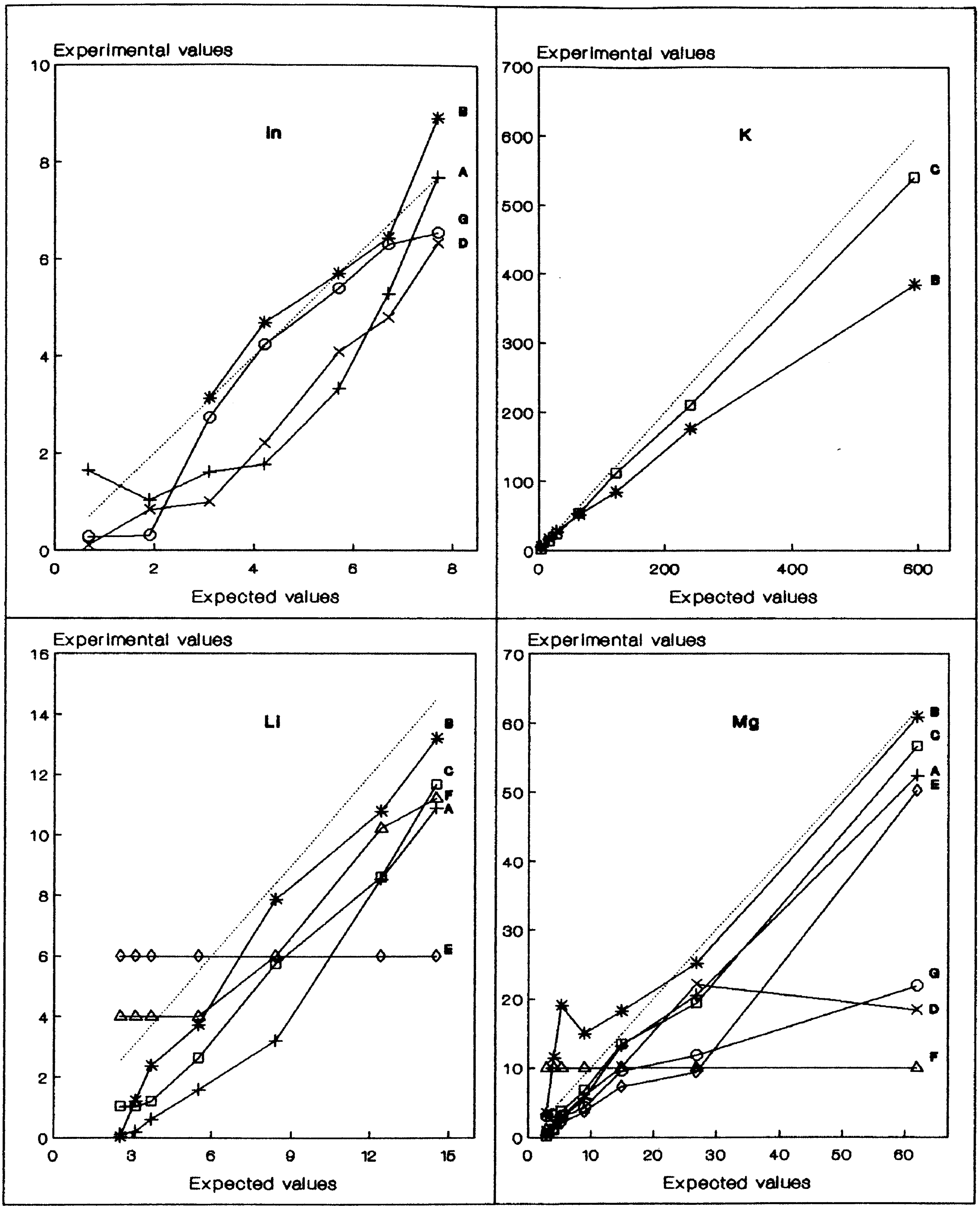
Laboratory	*Analytical Method*
A	*Inductively coupled plasma (ICP) optical emission spectroscopy (OES)*
B	*Spark-source mass spectrometry (SSMS)*
C	*Inductively coupled plasma (ICP) optical emission spectroscopy (OES)*
D	*Atomic absorption spectroscopy (AAS)*
E	*Arc emission spectroscopy (AES) (AgCl buffer)*
F	*Arc emission spectroscopy (AES) (NaCl buffer)*
G	*Direct current emission spectroscopy*

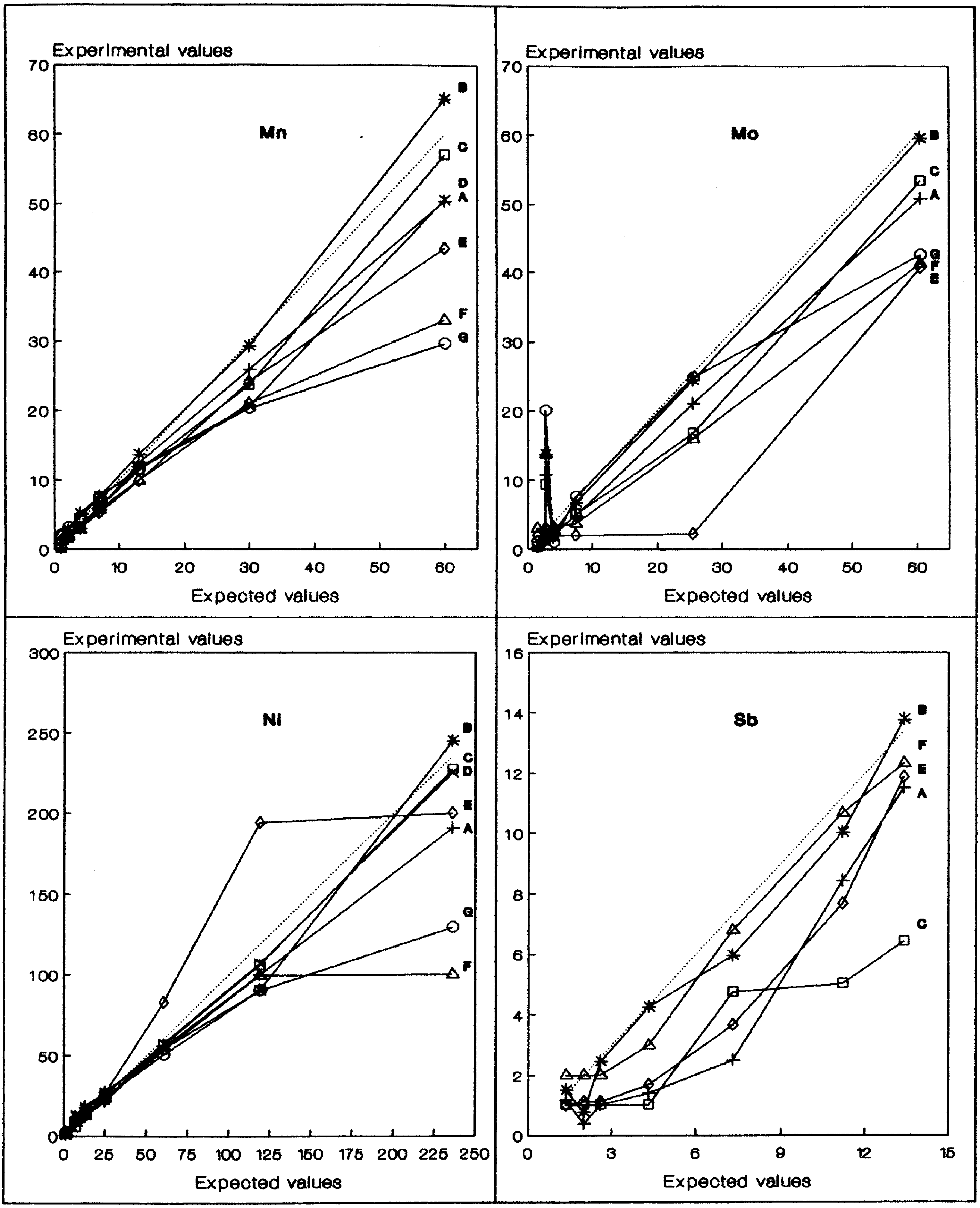
Experimental and expected values are given in the units μgX/gU. The dotted lines depict expected concentrations.

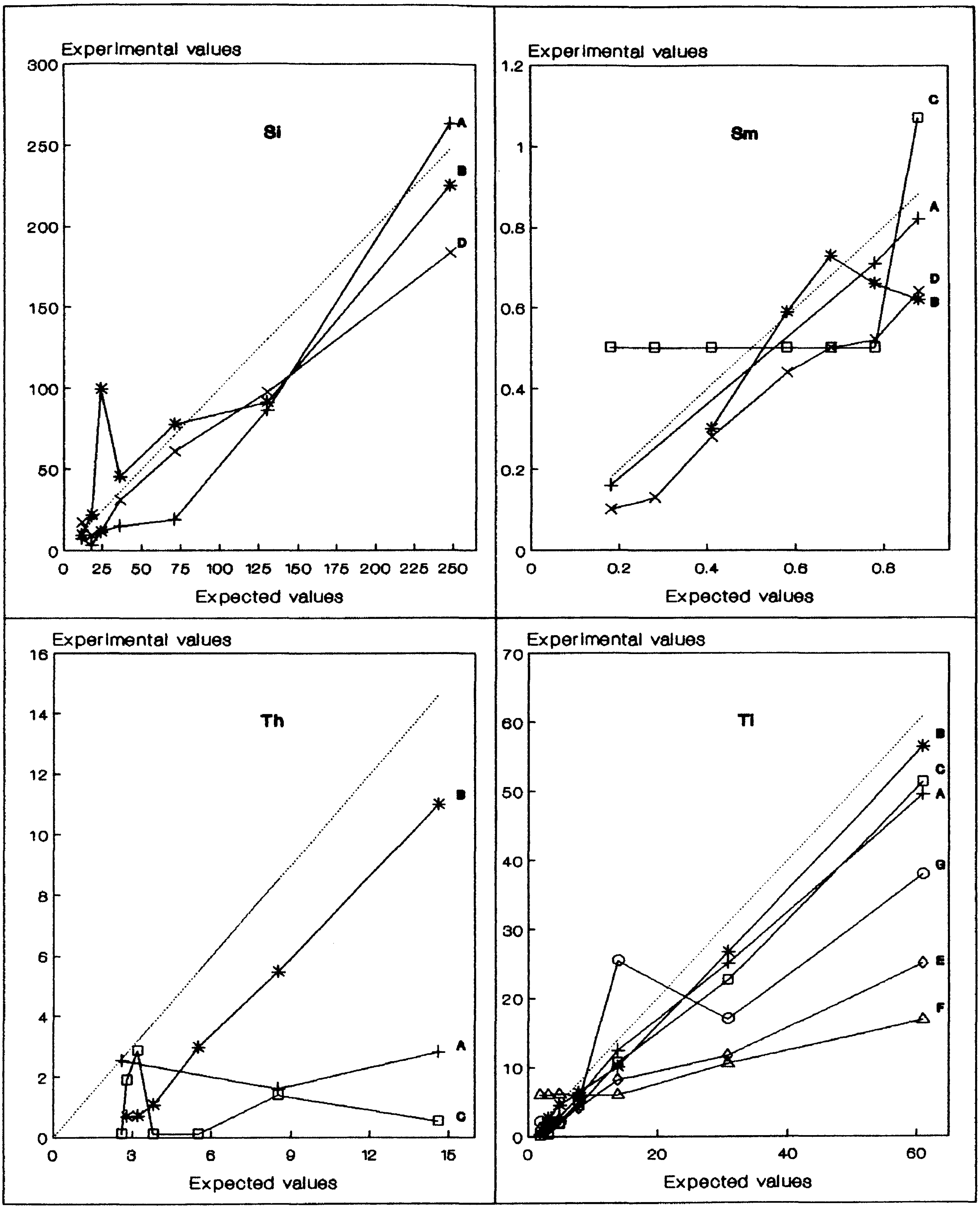

Experimental values
300
250
200
150
100
50
0
Al
D
B
A
C
G
E
F
0
50
100
150
200
250
Expected values
Experimental values
10
8
6
4
2
0
B
E
A
B
C
F
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
Expected values
Experimental values
20
15
10
5
0
Bi
D
B
F
A
G
E
0
3
6
9
12
15
Expected values
Experimental values
500
400
300
200
100
0
Ca
B
A
C
D
E
F
0
30
60
90
120
150
Expected values

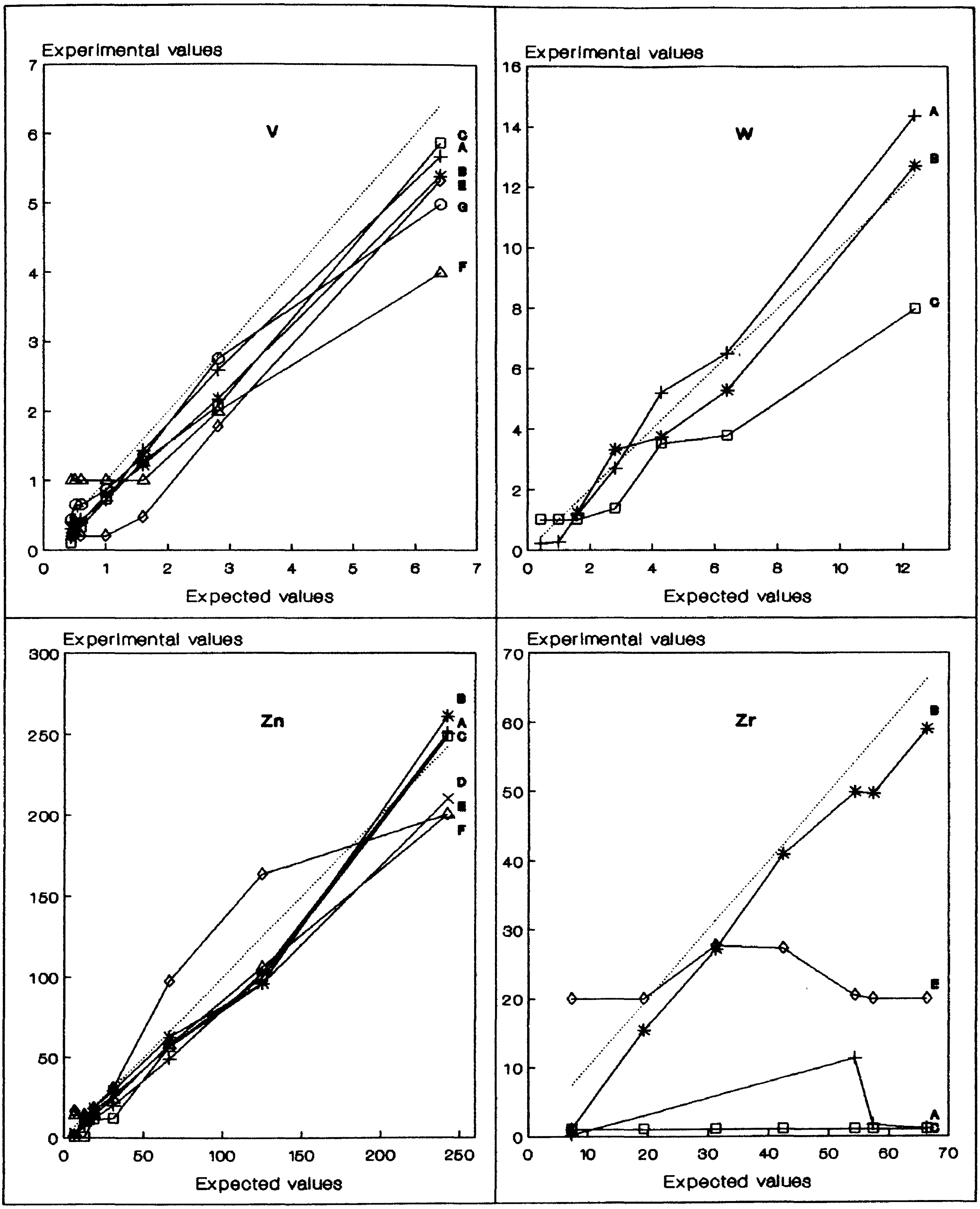

Experimental values
Cd
7
6
5
4
3
2
1
0
0
2
4
6
F
B
C
A
E
D
Expected values
Experimental values
Co
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
B
C
A
F
E
G
Expected values
Experimental values
Cr
200
150
100
50
0
0
20
40
60
80
100
120
B
A
C
G
F
E
Expected values
Experimental values
Cu
140
120
100
80
60
40
20
0
0
20
40
60
80
100
120
B
D
C
A
E
G
F
Expected values


Experimental values
1
0.8
0.6
0.4
0.2
0
Dy
D
B
A
C
0
0.2
0.4
0.6
0.8
Expected values
Experimental values
1
0.8
0.6
0.4
0.2
0
Eu
B
D
A
C
0
0.2
0.4
0.6
0.8
Expected values
Experimental values
1200
1000
800
600
400
200
0
Fe
G
B
A
C
D
F
E
0
150
300
450
600
750
900
Expected values
Experimental values
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Gd
A
B
C
D
0
0.2
0.4
0.6
0.8
1
Expected values


Experimental values
In
B
A
G
D
Expected values
0
2
4
6
8
10
Experimental values
K
C
B
Expected values
0
100
200
300
400
500
600
700
Experimental values
Li
B
C
F
A
E
Expected values
0
2
4
6
8
10
12
14
16
3
6
9
12
15
Experimental values
Mg
B
C
A
E
G
D
F
Expected values
0
10
20
30
40
50
60
70


Experimental values
Mn
Expected values
B
C
D
A
E
F
G
Experimental values
Mo
Expected values
B
C
A
G
F
E
Experimental values
Ni
Expected values
B
C
D
E
A
G
F
Experimental values
Sb
Expected values
B
F
E
A
C


Experimental values
Si
300
250
200
150
100
50
0
0
25
50
75
100
125
150
175
200
225
250
A
B
D
Expected values
Experimental values
Sm
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
C
A
D
B
Expected values
Experimental values
Th
16
14
12
10
8
6
4
2
0
0
3
6
9
12
15
B
A
C
Expected values
Experimental values
Ti
70
60
50
40
30
20
10
0
0
20
40
60
B
C
A
G
E
F
Expected values


Experimental values
V
7
6
5
4
3
2
1
0
0
1
2
3
4
5
6
7
Expected values
C
A
B
E
G
F
Experimental values
W
16
14
12
10
8
6
4
2
0
0
2
4
6
8
10
12
Expected values
A
B
C
Experimental values
Zn
300
250
200
150
100
50
0
0
50
100
150
200
250
Expected values
B
A
C
D
E
F
Experimental values
Zr
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
Expected values
B
E
A
D

CHAPTER FIVE

QUANTITATIVE ANALYSIS

5.1 *Calculation Methods*

The calculation method used to derive the formula for determination of relative sensitivity factors (RSF's) for impurity elements in different matrices relative to an internal standard is discussed in detail on page 138.

For clarity, the essential formulae are also given here:

$$\frac{Q_x}{Q_y} = \frac{K_x}{K_y} \cdot \frac{C_y}{C_x} \qquad \ldots\ldots\ldots\ldots\ldots (1)$$

where:

K_x/K_y is the RSF for element X relative to the internal standard, Y (see page 28).

Equation (1) can be rewritten as follows:

$$C_x = C_y \cdot \frac{\dfrac{K_x}{K_y}}{\dfrac{Q_x}{Q_y}} \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

where:

C_x is the unknown concentration of an element X,
C_y is the known concentration of the internal standard,

Q_x/Q_y is the ratio between the exposure values of an element X and the internal standard at 50% transmission, and

K_x/K_y is the relative sensitivity factor for element X relative to the internal standard, which is derived from calibration plots as the slope of the regression line.

Equation (1) can be used to determine the RSF of any element X relative to any internal standard (IS) in any matrix Z. Rewriting equation (1) into the above notation gives:

$$(RSF^{X}_{IS})_Z = \left[\frac{\dfrac{Q_X}{Q_{IS}}}{\dfrac{C_{IS}}{C_X}} \right]_Z \qquad \text{.........(3)}$$

This formula is directly related to the general formula for a RSF, namely:

$$RSF = \frac{C_{ms}}{C_{true}} \qquad \text{.........(4)}$$

where:

C_{ms} is the concentration of an element X relative to an internal standard determined experimentally with the mass spectrometer, and

C_{true} is the true concentration of an element X relative to an internal standard where both concentrations are known.

The calculation method used to derive the formula which is used to determine the unknown background concentration of an element X in different matrices, Z, using different standards is given below. The general spark-source mass spectrometry equation applies:

$$(C_X)_Z = \frac{K_X}{(Q_X)_Z} \qquad \text{.........(5)}$$

where:

$(C_X)_Z$ is the unknown concentration of element X in matrix Z,
K_X is a constant for element X, and
$(Q_X)_Z$ is the instrument signal for element X in matrix Z.

Equation (5) also applies when a known standard (STD) is added to the matrix Z:

$$(C_X)_{Z+std} = \frac{K_X}{(Q_X)_{Z+std}} \qquad \text{.........(6)}$$

where:

$(C_X)_{Z+std}$ is the unknown concentration of element X in the matrix Z plus the known concentration of element X in the standard,
K_X is a constant (see equation (5)), and
$(Q_X)_{Z+std}$ is the combined instrument signal for element X and the standard in the matrix Z.

In order to determine the unknown background concentration $(C_X)_Z$ of element X in matrix Z, equations (5) and (6) are combined as follows:

$$(C_X)_{Z+std} - (C_X)_Z = K_X \left[\frac{1}{(Q_X)_{Z+std}} - \frac{1}{(Q_X)_Z} \right]$$

This difference is equal to the concentration of the added standard, expressed as $(C_X)_{std}$:

$$(C_X)_{std} = K_X \left[\frac{(Q_X)_Z - (Q_X)_{Z+std}}{(Q_X)_{Z+std} \cdot (Q_X)_Z} \right] \qquad \ldots\ldots\ldots(7)$$

$(Q_X)_Z$ and $(Q_X)_{Z+std}$ values can be determined as outlined on page 105 below.

$(C_X)_{std}$ values are known and K_X can be calculated. Inserting the K_X value for element X in equation (5) enables the determination of $(C_X)_Z$. This leads to the following equation:

$$(C_X)_Z = (C_X)_{std} \cdot \frac{(Q_X)_{Z+std}}{(Q_X)_Z - (Q_X)_{Z+std}} \qquad \ldots\ldots\ldots(8)$$

Equation (8) is the fundamental formula used to determine the background concentration of an element X in a matrix Z, using known prepared graphite standards. This formula will be used to determine background concentrations of impurity elements in U_3O_8 and UF_4 matrices in the following sections. The instrument signals of element X in both the matrix Z and the combination of matrix plus standard can be expressed relative to an internal reference standard (IS) (see page 28). Q_{IS} values are the same in the Z and Z+STD matrices for a particular choice of Y concentration.

Equation (8) then converts to:

$$(C_X)_Z = (C_X)_{std} \cdot \frac{(Q_X/Q_{IS})_{Z+std}}{(Q_X/Q_{IS})_Z - (Q_X/Q_{IS})_{Z+std}} \qquad \ldots\ldots\ldots(9)$$

This formula only holds true when $(Q_X/Q_{IS})_Z$ is larger than $(Q_X/Q_{IS})_{Z+std}$. The opposite can never happen in spark-source mass spectrometry because the concentration is inversely proportional to the instrument signal. Thus, the higher the concentration, i.e. when the standard is added to the matrix Z, the resultant instrument signal will be smaller than that for only the matrix Z.

5.2 U_3O_8/graphite matrix quantitation

5.2.1 Blank correction

In order to determine relative sensitivity factors (RSF's) for impurity elements in a U_3O_8/graphite matrix, the blank U_3O_8 sample must first be quantified. Considerable effort was initiated to obtain a blank U_3O_8 sample with few impurity elements to ensure a background spectrum relatively free from spectral lines. This blank base U_3O_8 sample (ES 0) was then mixed with a graphite powder, spiked with Y as an internal reference standard, in the ratio of five parts U_3O_8 to one part graphite by mass. The choice of this ratio has been discussed on page 30. The sample was then analysed several times to obtain an instrument signal, $(Q_X/Q_{\bar{Y}})_{U_3O_8}$ for element X relative to the internal standard, Y, in a U_3O_8/graphite matrix. The exposure value for Y, $Q_{\bar{Y}}$, is the mean of the singly and doubly charged species. The blank base U_3O_8 sample used for this purpose is stoichiometric i.e. 100 per cent U_3O_8.

To be able to quantify the impurity elements present in the blank base U_3O_8 sample, a range of graphite standards were prepared which contained the impurity elements under investigation in different concentrations, together with Y as internal reference standard. The method followed to prepare these graphite standards has been described on page 26. UCAR SP1 graphite powder was used for these standards. The concentration range of the standards is as follows:

U_3O_8 used: stoichiometric i.e. 84,8 per cent U.

Concentrations: 4 µg X /gC
20 µg X /gC
40 µg X /gC
100 µg X /gC
200 µg X /gC

Expressed relative to U, the concentrations $(C_x)_{std}$ for each impurity element X, become:

1 µg X /gU
5 µg X /gU
10 µg X /gU
25 µg X /gU
50 µg X /gU

The concentration of Y added to each of the above graphite standards as internal standard is 20 µg Y/gC or 5 µg Y/gU.

In addition to the above range of graphite standards using UCAR SP1 graphite, a range of check standards were also prepared using Ultra 'F' graphite. The main reason for preparing these check standards was to see whether results obtained for certain elements using UCAR SP1 graphite could not be improved by using Ultra 'F' graphite. The difference between these two graphite powders' background spectra for certain elements was used to check the results obtained from the UCAR SP1 range of graphite standards. This was especially useful for Fe, which has a high background concentration in UCAR SP1 compared to Ultra 'F'. Additional impurity elements not incorporated in the UCAR SPI graphite standards were now added to these check standards using Ultra 'F' graphite. These elements could not be added to the UCAR SP1 graphite because of spectral line interferences from elements already added. However due to the absence of these interfering elements in Ultra 'F' graphite these additional impurity elements could be added and analysed without any interference. Elements falling into this category were Li, W, P, Na, K and S. This fact also accounts for the low value for the number of analyses in Table 5.2 (see page 111) where the calibration curve parameters are listed.

The concentration range of these check graphite standards is as follows:

Concentrations: 20 μg X /gC
40 μg X /gC
80 μg X /gC
200 μg X /gC

Expressed relative to U, the concentration, $(C_x)_{std}$, becomes:

5 μg X /gU
10 μg X /gU
20 μg X /gU
50 μg X /gU

The concentration of Y added to each of the above graphite check standards as internal standard is 80 µgY/gC or 20 µgY/gU.

Using standard addition methods, each of the above graphite standards are mixed with the blank base U_3O_8 *sample in the ratio of five parts* U_3O_8 *to one part graphite by mass. Similarly, as for the blank base* U_3O_8*/graphite matrix sample, each sample is analysed several times to obtain an instrument signal,* $(Q_x/Q_y^-)_{U_3O_8+std}$*, for element X relative to the internal standard in the blank base* U_3O_8 *plus the graphite standard. These instrument signals are used in equation (9) to calculate the concentration of element X in the blank base* U_3O_8*,* $(C_x)_{U_3O_8}$

$$(C_x)_{U_3O_8} = (C_x)_{std} \frac{(Q_x/Q_y^-)_{U_3O_8+std}}{(Q_x/Q_y^-)_{U_3O_8} - (Q_x/Q_y^-)_{U_3O_8+std}}$$

The results obtained to quantify the impurity elements in the blank base U_3O_8 *sample are given in Table 5.1 as* C_x*(SSMS) in µgX /gU.*

The concentration values for Na (20,9), Mg (26,0), Si (18,3) and Fe (20,3) are all very high in comparison to the concentrations of the graphite standards e.g. the 1, 5, 10 and 25 µgX/gU standards. This fact greatly influences the gradient of the calibration line. This is shown as follows:

On the x-axis of the calibration curve, the ratio C_y/C_x *is plotted where* $C_x = (C_x)_{std} + (C_x)_{U_3O_8}$*. Thus when* $(C_x)_{U_3O}$ *is large, the ratio* C_y/C_x *becomes smaller where* C_y *is taken as constant. This makes the gradient, m, of the regression line*

Table 5.1: Blank Base U_3O_8 (ES 0) quantification

Element	Charge State(+)	n	Std Error at 95 % CL (%)	C_x (SSMS) (µg X /gU)	Certified conc (µg X /gU)
B	1	18	10,4	9,8	0,07
Na	1	5	42,1	20,9	5
Mg	2	12	31,2	26,0	0,5
Al	2	18	13,3	9,6	1
Si	2	16	33,6	18,3	17
P	1 & 2	12	18,4	3,5	-
Ca	2	35	16,1	6,0	2,2
K	1 & 2	6	25,2	5,6	4
Ti	1 & 2	14	12,6	0,42	0,3
V	1 & 2	38	18,0	0,38	0,31
Cr	1 & 2	45	10,0	5,3	2
Mn	1 & 2	34	12,6	0,35	0,14
Fe	1 & 2	22	9,7	20,3	13
Co	1 & 2	26	8,1	0,30	0,1
Ni	1	28	10,5	2,4	0,8
Cu	1 & 2	26	12,3	0,5	0,3
Zn	1	31	7,3	1,78	1,66
Zr	1 & 2	36	12,9	3,5	0,5
Mo	2	12	18,7	2,5	0,3
Sb	1	25	14,1	1,22	1,2
Li	1	3	19,3	0,19	0,21

inaccurate and limits the calibration range. In this way the RSF is influenced directly by a high background concentration. Even elements with lower background concentrations e.g. B (9,8) and Al (9,6) influence the Q-values of the lower graphite standards with concentrations of 1, 5 and 10 µgX/gU. The same can be said for Ca (6,0), K (5,6) and Cr (5,3) which influence the two lowest graphite standards with concentrations of 1 and 5 µgX/gU. The rest of the elements in Table 5.1 have background concentrations which do not influence the calculation of relative sensitivity factors significantly.

The C_x *values in Table 5.1 determined for impurity elements in the blank base* U_3O_8 *are only for the elements in their elemental state. The hydrogenated and oxygenated species of the elements have not been considered. When analysing unknown* U_3O_8 *samples with the spark-source mass spectrometer, it is assumed that the same degree of hydrogenation and oxygenation of elements in the sample takes place as with the* U_3O_8 *calibration standard samples. This assumption is reasonable if the unknown sample is also stoichiometric* U_3O_8 *and the sparking parameters used to generate ions are identical for the* U_3O_8 *sample as for the* U_3O_8 *calibration standard samples.*

The chemical composition of the impurity elements within the U_3O_8 *samples are also assumed to be similar to those in the* U_3O_8 *calibration standard samples. The plasma generated between the two electrodes in the ion source provides the equalising locality for such differences. In this plasma the chemical structures are atomised and ionised and recombination of species takes place.*

The high standard errors at 95% confidence level (CL) for Na (42,1%) and K (25,2%) can be ascribed to the small number of data points (n = 5 for Na and n = 6 for K). The fact that the concentration of Na in the blank base U_3O_8 sample is quite high (C_x = 20,9 µg Na/gU) also plays a direct role in the relatively high uncertainty.

Similarly, the high standard errors at 95% CL for Mg (31,2%) and Si (33,6%) can also be ascribed to the high concentrations of these two elements in the blank base U_3O_8 sample (C_x = 26,0 for Mg and C_x = 18,3 for Si). This explains why the $(C_x)_{U_3O_8}$ values for these two elements fluctuated over the concentration range of the graphite standards. This fluctuation can further be enhanced by the position on the photoplate where the spectral lines of Mg at m/e 12,5 and of Si at m/e 14,5 are influenced by background emulsion fogging due to the strong spectral line of the major component, ^{12}C at m/e 12. This interference directly affects the results obtained for Mg and Si and can lead to large standard errors.

For the remainder of the impurity elements in the blank base U_3O_8 sample, the standard errors at a 95% CL show typical values comparable to the precision of the method, namely approximately 20%. The large values of n for these elements also ensures the reliability of the lower $(C_x)_{U_3O_8}$ values over the concentration range of the graphite standards.

In Table 5.1 concentration values of impurities in the base U_3O_8 material obtained with the spark-source mass spectrometer are compared with values obtained using different analytical techniques (see certified concentration column). These techniques are described on page 158. The main reason for some of the differences is the fact that the C_x (SSMS) values include the concen-

tration of that particular element present in the graphite powder used. In other words, the C_x (SSMS) value reported is a combination of the concentration of that particular element in the blank base U_3O_8 sample as well as the concentration of that particular element in the UCAR SP1 graphite or Ultra 'F' graphite used. In this way, the impurities in the graphite powder have been quantified and should be kept in mind when using these graphite powders for future analyses.

Differences can also be due to contamination picked up from a variety of sources. An important source of contamination, especially at trace level concentrations, is from ordinary dust in the laboratory environment [24]. Typical elements found in dust samples collected in the laboratory and analysed for impurities included such elements as B, Mg, Al, Si and Ca. It has also been shown that the Na from NaCl in human perspiration is a significant source of Na contamination. Another source of contamination is from the stainless steel tools which are used in the preparation of the electrodes. Possible impurity elements include Al, Cr, Fe, Ni, Zr and Mo. It is thus difficult at this stage to identify the exact sources of contamination and to quantify these impurities. Proposals to prevent or minimise such contamination are discussed in Chapter 7 on page 166.

5.2.2 Calibration Curves

Calibration curves are constructed according to equation (1) on page 98. Q_x/Q_y is plotted on the y-axis. The value of C_x in C_y/C_x is taken as the sum of the concentrations of an element X in the prepared graphite standard plus the value in the blank base U_3O_8. Expressed as symbols, $C_x = C_{std} + C_{U_3O_8}$ where $C_{U_3O_8}$ is obtained from Table 5.1 on page 106.

The slope, K_x/K_y, of the calibration curve is the relative sensitivity factor (RSF) of that particular impurity element X present in the matrix U_3O_8 relative to an internal standard, Y. Calibration curve parameters are listed in Table 5.2 . The parameters c, r and n are discussed below. The standard error, s_m, in the slope is expressed in the form of the confidence limits of the slope, α, at a 95% confidence level (CL). These two parameters are discussed on pages 115 and 148 in terms of the statistical significance of the results.

The values of the intercept on the y-axis (c) are, with only a few exceptions, relatively close to the origin (0;0). The value of c must be evaluated in perspective with the magnitude of the scale of the y-axis. Elements with high RSF's have large absolute values for c. Examples of such elements are K^{2+} ($c = -0{,}6448$) and Bi^{2+} ($c = -1{,}0788$). Furthermore, elements with large α's also tend to have large values for c. This follows from the uncertainty in the slope of the regression line. Elements classified into this category are Mo^{1+} and W^{2+}. The intercept on the y-axis is reflected in the correlation coefficient of the fit of data to a regression line. A bad fit suggests that there are unreliable data points which, when included, would affect the intercept on the y-axis. Elements falling into this category are Mo^{1+} and Ba^{1+}. The value of c is not of importance as it is not incorporated directly into any calculations regarding concentration or RSF's.

However, the value obtained for r is an indication of the fit of the data to the regression line. Ideally, r should be unity. The values of r obtained in Table 5.2 are generally quite good. The rather poor fits of data for Fe^{1+} ($r = 0{,}8529$), Ba^{1+} ($r = 0{,}8972$) and Mg^{2+} ($r = 0{,}9278$) are also apparent from the

Table 5.2: U_3O_8 Calibration curve parameters

Element	Charge State(+)	m (RSF)	a (%)	c	r	n
B	1	1,1468	4,6	-0,0122	0,9961	19
Na	1	0,2483	28,2	0,0016	0,9716	7
Mg	2	1,7725	19,3	-0,0898	0,9278	21
Al	2	1,2399	10,9	0,0083	0,9740	22
Si	2	1,2836	15,1	-0,0197	0,9273	32
P	1	0,2178	20,8	0,0121	0,9839	7
P	2	1,3978	37,8	0,0511	0,9649	6
Ca	2	0,3035	12,2	-0,0216	0,9317	44
K	1	0,1073	15,7	-0,0014	0,9883	8
K	2	18,3676	24,2	-0,6448	0,9910	5
Ti	1	0,2598	16,0	0,0004	0,9660	15
Ti	2	0,4684	5,3	-0,0061	0,9969	12
V	1	0,3025	2,4	0,0248	0,9955	24
V	2	0,5004	19,9	0,0489	0,9580	13
Cr	1	0,2408	9,9	0,0087	0,9622	36
Cr	2	0,7199	9,4	-0,0082	0,9847	18
Mn	1	0,1529	10,3	0,0357	0,9753	23
Mn	2	1,0094	17,8	0,0324	0,9660	13
Fe	1	0,2301	23,6	0,0041	0,8529	30
Fe	2	1,1867	13,1	-0,0039	0,9809	13
Co	1	0,2697	4,0	-0,0049	0,9957	25
Co	2	1,2153	12,9	0,0362	0,9836	12
Ni	1	0,2397	5,7	0,0099	0,9898	29
Cu	1	0,2987	7,3	0,0215	0,9840	28
Cu	2	3,9934	8,2	0,0669	0,9924	13
Zn	1	0,6078	7,4	0,0074	0,9857	25
Sr	1	0,4877	10,0	0,1405	0,9767	23
Sr	2	0,3316	11,7	0,0109	0,9848	13

Table 5.2: Continued

Element	Charge State(+)	m (RSF)	α (%)	c	r	n
Zr	1	1,3375	7,8	0,0501	0,9839	25
Zr	2	0,6769	8,9	-0,0154	0,9911	13
Nb	1	1,3581	8,5	0,0273	0,9814	25
Nb	2	0,9780	10,1	-0,0180	0,9886	13
Mo	1	2,8176	19,2	-0,3758	0,9249	22
Mo	2	1,4294	9,1	-0,0468	0,9907	13
Ru	1	2,8572	6,0	-0,0171	0,9927	20
Ru	2	5,1368	19,2	0,0095	0,9609	13
Cd	1	1,1031	13,2	0,1175	0,9702	25
In	1	0,5853	12,5	0,1331	0,9607	25
In	2	7,7360	11,9	0,0027	0,9842	13
Sb	1	1,7565	16,9	0,0113	0,9342	24
Sb	2	7,0408	7,5	-0,1386	0,9937	13
Ba	1	0,5416	23,0	0,6769	0,8972	22
Ba	2	0,4784	10,5	0,0230	0,9879	13
Sm	1	4,2008	45,0	0,0000	0,9310	7
Sm	2	0,6019	4,9	0,0437	0,9945	26
Eu	1	4,6455	6,2	0,0082	0,9962	12
Eu	2	0,6633	9,7	0,0179	0,9743	26
Gd	1	3,6455	7,4	-0,0127	0,9960	12
Gd	2	0,9391	5,5	-0,0087	0,9939	20
Dy	1	7,2053	6,3	-0,1353	0,9960	12
Dy	2	0,6998	5,5	0,0883	0,9922	24
W	2	2,1239	40,3	0,5395	0,9604	6
Bi	2	20,1841	14,8	-1,0788	0,9681	16
Th	2	2,0486	7,7	-0,0852	0,9889	19
Li	1	0,0243	7,1	0,0002	1,0000	5

large errors in the slopes where α for Fe^{1+} = 23,6%, α for Ba^{+} = 23,0% and α for Mg^{2+} = 19,3%. Another explanation for the poor calibration lines for Fe^{1+} and Mg^{2+} is the high values of these elements in the blank base U_3O_8, where $C_{U_3O_8} = 20,3$ µg Fe/gU for Fe^{1+} and $C_{U_3O_8} = 26,0$ µg Mg/gU for Mg^{2+}. This is in spite of the large number of data points (n) used to draw the calibration curves for these elements. The calibration graph for Fe^{1+} in a U_3O_8 matrix is given in Figure 5.1 as an example of a poor calibration curve.

Good calibration curves were obtained for Co^{1+} and V^{1+} as indicated by the correlation coefficients obtained for these elements where r = 0,9957 and r = 0,9955, respectively. Factors contributing to the good fit of data points for these elements is the fact that they both have very small α values where α = 4,0% for Co^{1+} and α = 2,4% for V^{1+}. Another reason is the fact that they both have small concentrations in the blank base U_3O_8 where $C_{U_3O_8} = 0,3$ µgCo/gU for Co^{1+} and $C_{U_3O_8} = 0,38$ µgV/gU for V^{1+}. In both cases the value of n is large where n = 25 for Co^{1+} and n = 24 for V^{1+}. A typical example of a good calibration curve is given in Figure 5.2 for Co^{1+} in a U_3O_8 matrix. Another good calibration curve is obtained for B^{1+} where the concentration obtained in the blank base U_3O_8 is fairly high where $C_{U_3O_8} = 9,8$ µgB/gU for B^{1+}. The other parameters coupled to this calibration curve are: r = 0,9961; n = 19 and α = 4,6%. This calibration line is also given in Figure 5.3 as a good line where a large background concentration is present.

The value of n in Table 5.2 is the number of data points where each analysis was taken as a separate data point. The value for the blank is also incorporated in n as a data point.

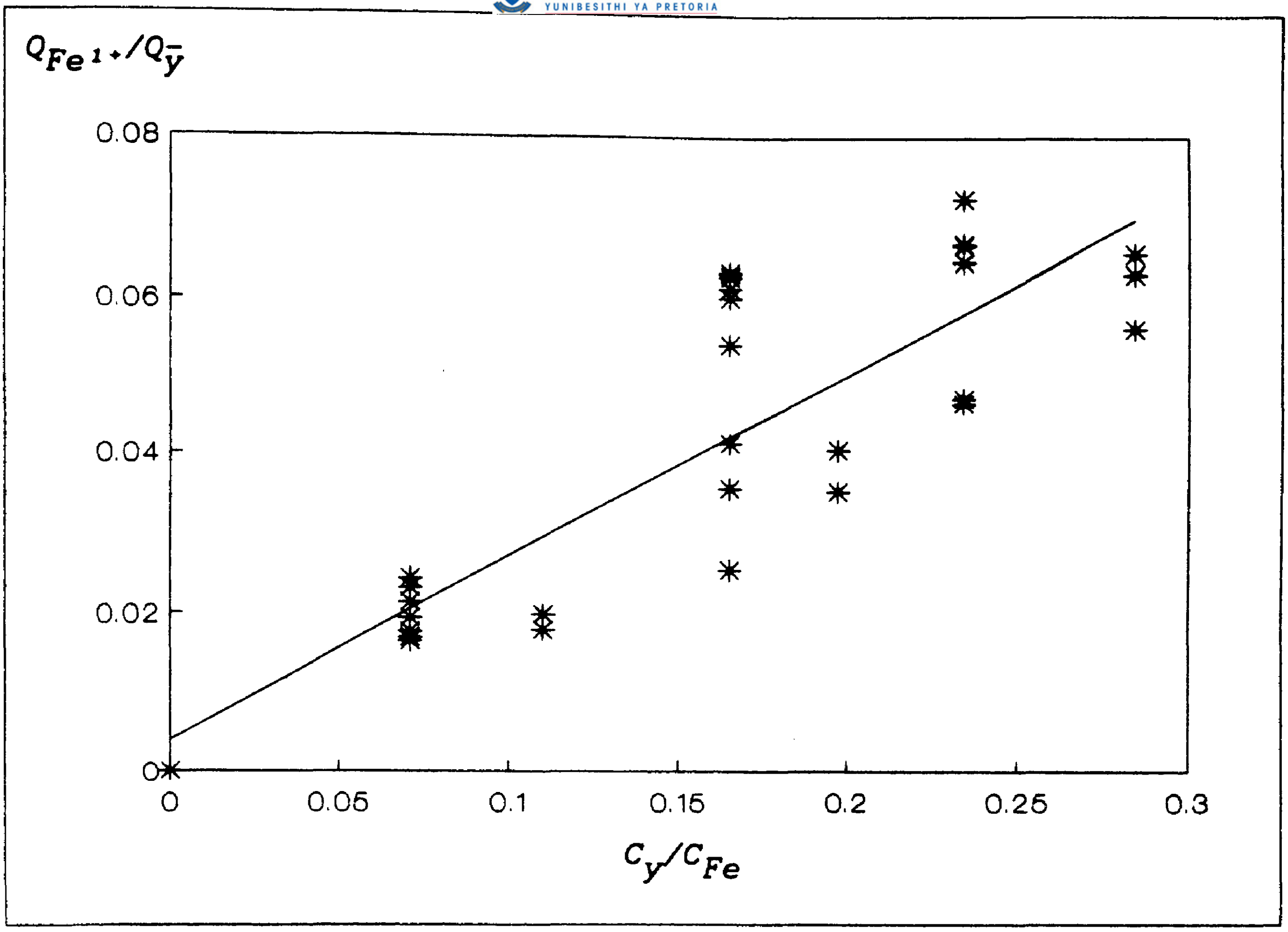


Figure 5.1: Calibration curve for Fe^{1+} in a U_3O_8/graphite matrix

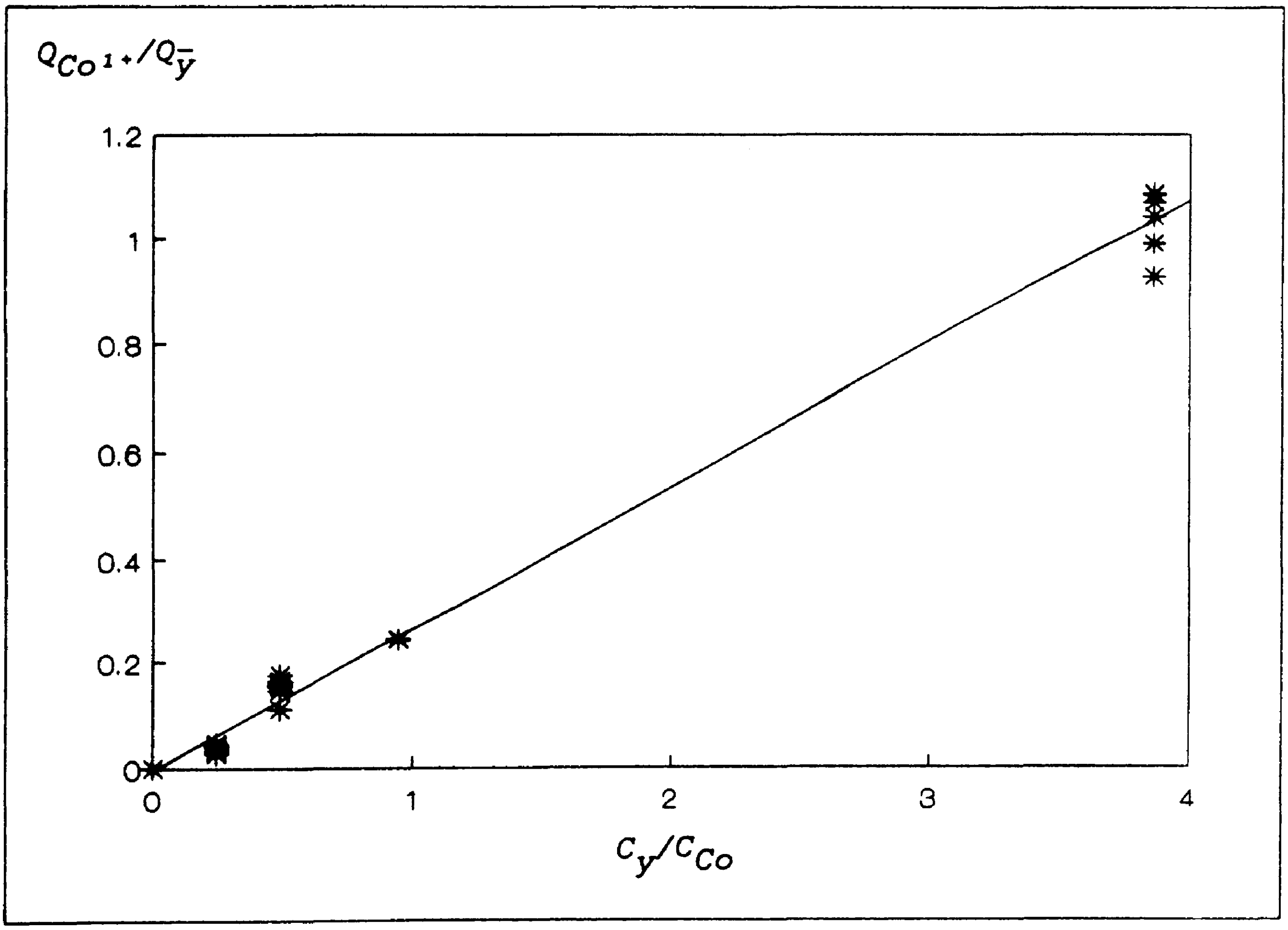


Figure 5.2: Calibration curve for Co^{1+} in U_3O_8/graphite matrix

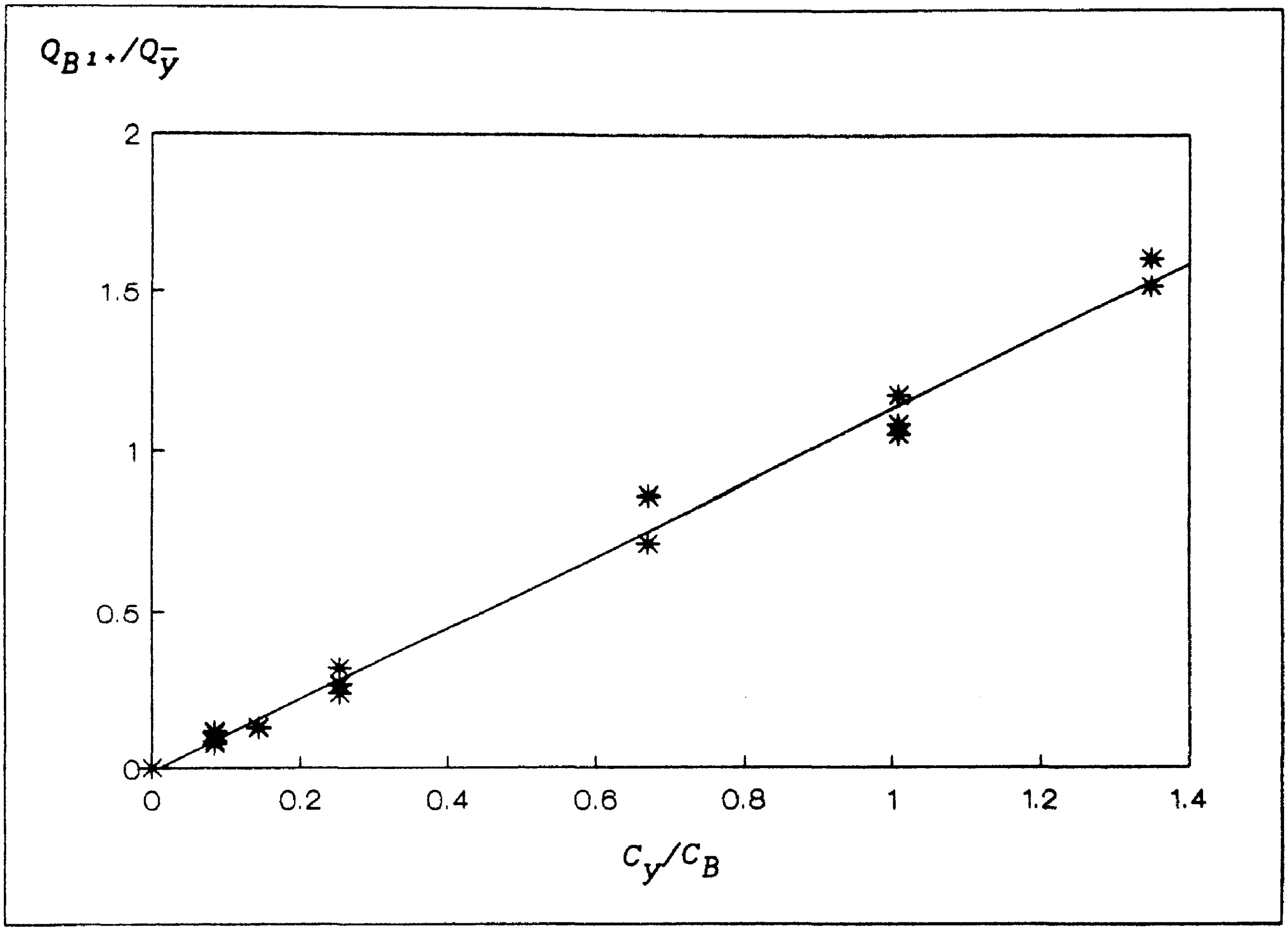


Figure 5.3: Calibration curve for B^{1+} in a U_3O_8/graphite matrix

5.2.3 Relative sensitivity factors (RSF's) - U_3O_8

The instrument sensitivity for a particular element is totally unique for a specific spark-source mass spectrometer and detection system. Different RSF's will be obtained for an element using a radio frequency (RF) spark compared to a triggered low-voltage discharge spark as was used in this investigation.

Another important factor to be considered is that a RSF for a particular element X will differ from matrix to matrix [25]. This is illustrated when comparing RSF's obtained for mutual elements (e.g. Al, P, Ca, Si and Zn) for both a UF_4 and a U_3O_8 matrix. Differences in this case could be ascribed, among other reasons, to the fact that in a UF_4 matrix, fluorination occurs within the plasma resulting in less elemental species of ions.

A RSF is also unique with regard to a particular internal reference standard.

It was beyond the scope of this investigation to determine whether a RSF for an element in a U_3O_8 *matrix will differ from that for another uranium oxide matrix, for example* UO_2 *or* UO_3*. It is the author's opinion that there would not be a significant difference because the combinations of uranium and oxygen would create very similar plasma conditions [11]. In all uranium oxide matrices, there is an over-abundance of oxygen species generated within the plasma.*

Correlations between physico-chemical properties of various elements as impurities and relative sensitivity factors have been published [23, 26]. Instead of using standards to determine RSF's, some authors have determined theoretical RSF's from making use of various combinations of physico-chemical properies of the elements. For the purpose of this investigation, an attempt will only be made to explain certain of the anomalies observed in the experimentally determined RSF's.

Physico-chemical properties such as heats of vaporisation, electrical resistivity, thermal conductivity, ionisation potentials, atomic radii and melting points were studied and some correlations drawn. These correlations are qualitative at their best. Due to the complexity of plasmas in relation to the physico-chemical properties, anomalies cannot be adequately explained in this qualitative fashion. It would require computer simulations involving chemical and physical studies in order to relate the properties to RSF's. This is a very complex task which has not been described in the literature and is beyond the scope of this thesis. Qualitative comments will nevertheless be offered for some of the observations.

The high relative sensitivity factors (RSF's) obtained for a few of the impurity elements in a U_3O_8/graphite matrix can be related to their physico-chemical properties with some degree of confidence. Elements which do not readily form ions of a particular species tend to have high RSF's for this species. A prime example is K^{2+} which has a very low ion yield for doubly charged species. A factor in this regard is the fact that potassium has only one valence electron in its outermost shell (4s orbital). This valence electron is readily lost to form the singly charged state having the noble gas structure of argon. Thereafter, it would require far more energy to remove a second electron to form the doubly charged species. This fact could be related to the second ionisation potential (I_P^{II}) for K which, together with the other alkali-earth metals, has the highest I_P^{II} of all the elements. The RSF of 18,3676 obtained for K^{2+} differs considerably from that obtained for K^+ (RSF = 0,1073). It is evident that K^+ ions are formed in great abundance in the mass spectrometer. Another element which has a small RSF is Li (RSF = 0,0243). Both Li and K are alkali-earth metals of group IA which readily lose an electron to have a noble gas structure. In the case of Li, this would be helium. Na also has a relatively small RSF namely 0,2483. All the group IA elements have of the lowest melting points which would contribute to the high yield of ions for these elements and the subsequent low RSF's. These elements also have of the lowest electrical resistivity of all the elements present. This fact could also contribute to these elements being atomised and ionised more easily.

Bismuth has a high electrical resistance which could account for the very poor ion yield for the Bi^{2+} ion and the subsequent high RSF value. Only the doubly charged Bi^{2+} was recorded (see page 71). Bismuth is also the most diamagnetic of all the metals and the thermal conductivity is lower than any metal, except for Hg. Both the electrical resistivity and the thermal conductivity are physico-chemical properties which play a role in the generation of the plasma between the two electrodes in the ion-source.

Another group of elements having relatively high RSF's are the singly charged species of the rare-earth metals e.g. Sm, Eu, Gd and Dy. These all have relatively high electrical resistivities and large atomic radii. It was found that the ion yield for doubly charged species was greater than for the singly charged species. This can be demonstrated by plotting the number of ions yielded against the charge state [27].

It would seem that the larger the atom becomes, the fewer ions reach the photoplate, probably due to their momentum and collisions in the flight tube. Elements falling into this category are W^{2+}, Th^{2+}, Sb^{2+}, In^{2+}, Ru^{2+}, Ru^{1+} and Mo^{1+}, and high RSF's could be expected. However, it should be taken into account that the number of ions generated in the ion source also plays a determining role.

The relatively high RSF for Cu^{2+} (RSF = 3,9934) is of interest as it is the highest of the 3d transition elements. Cu and Ag have of the lowest electrical resistance as well as the highest thermal conductivity. They both are group IB elements having electron configurations such that their d-orbitals are filled and having one electron in the outermost s-orbital. The filled d-orbitals lead to stability and an electron is readily lost from the half filled s-orbital. In order to lose another electron to form Cu^{2+} species, more energy is required to remove an electron from a paired 3d orbital resulting in a high RSF for Cu^{2+}.

Only a few of the physico-chemical properties of the elements have been referred to in order to explain some of the anomalies obtained with RSF's for impurities in a U_3O_8/graphite matrix. Properties such as bond strengths in diatomic molecules and heats of formation of gaseous atoms from elements in their standard states should also be included when attempting to explain these anomalies.

The RSF's obtained from calibration curves can be checked by making use of the instrument signals obtained. The ratio between the instrument signal for the singly charged state of an element and the instrument signal for the doubly charged state of the same element at a concentration level should be the same as the ratio between the RSF of the singly charged state of the particular element and the RSF for the doubly charged state of that element. The ratio X^{1+}/X^{2+} is independent of the concentration of element X. A number of elements were measured both in the singly and doubly charged states at two different concentration levels. The means of the ratio X^{1+}/X^{2+} between these two concentrations were compared and good correlation was obtained. This ratio was used to test the ratio RSF X^{1+}/RSF X^{2+} for the same element using the RSF's obtained in Table 5.3. Good agreement was obtained for most of the elements, which confirmed that outliers did not seriously influence the determination of RSF's. The ratio X^{1+}/X^{2+} can be used with a RSF for X^{1+} to get an estimate of the RSF for X^{2+} and vice versa.

Table 5.3: Relative Sensitivity Factors: U_3O_8/Graphite Matrix

RSF Singly charged Species	Element	RSF Doubly charged Species	$\frac{RSF\ X^{1+}}{RSF\ X^{2+}}$	X^{1+}/X^{2+} $C_x=10\mu gX/gU$	X^{1+}/X^{2+} $C_x=50\mu gX/gU$
0,0243	Li				
1,1468	B				
0,2483	Na				
	Mg	1,7725			
	Al	1,2399			
	Si	1,2836			
0,2178	P	1,3978			
	Ca	0,3035			
0,1073	K	18,3676			
0,2598	Ti	0,4684			
0,3025	V	0,5004	0,60	0,60	0,58
0,2408	Cr	0,7199	0,33	0,34	0,37
0,1529	Mn	1,0094	0,15	0,15	0,15
0,2301	Fe	1,1867	0,19	0,20	0,20
0,2697	Co	1,2153	0,22	0,22	0,21
0,2397	Ni				
0,2987	Cu	3,9934	0,07	0,08	0,09
0,6078	Zn				
0,4877	Sr	0,3316	1,47	1,55	1,85
1,3375	Zr	0,6769	1,98	2,03	2,06
1,3581	Nb	0,9780	1,39	1,42	1,27
2,8176	Mo	1,4294	1,97	2,02	2,02
2,8572	Ru	5,1368	0,56	1,37	0,67

Table 5.3: Continued

RSF Singly charged Species	Element	RSF Doubly charged Species	$\frac{RSF\ X^{1+}}{RSF\ X^{2+}}$	X^{1+}/X^{2+} C_x=10µgX/gU	X^{1+}/X^{2+} C_x=50µgX/gU
1,1031	Cd				
0,5853	In	7,7360	0,08	0,08	0,09
1,7565	Sb	7,0408	0,25	0,25	0,24
0,5416	Ba	0,4784	1,13	1,08	1,19
4,2008	Sm	0,6019	6,98	6,63	6,55
4,6455	Eu	0,6633	7,00	7,05	7,58
3,6455	Gd	0,9391	3,88	3,97	3,89
7,2053	Dy	0,6998	10,30	10,64	9,76
	W	2,1239			
	Bi	20,1841			
	Th	2,0486			

5.3 UF_4-graphite matrix quantitation

5.3.1 Blank correction

In order to determine relative sensitivity factors (RSF's) for impurity elements in a UF_4/graphite matrix, the blank UF_4 sample which was to be used to simulate the matrix material first had to be quantified. Considerable effort was initiated to obtain a blank UF_4 sample with the least impurity elements to ensure a background spectrum relatively free from spectral lines. This blank UF_4 sample was mixed with graphite powder, spiked with Y as an internal reference standard, in the ratio of one to one by mass. The sample was then analysed several times to obtain an instrument signal $(Q_x/Q_{\bar{y}})_{UF_4}$ for element X relative to the internal standard, Y. The exposure value for Y, $Q_{\bar{y}}$, is the mean for the singly and doubly charged species. The blank UF_4 sample used for this purpose is stoichiometric i.e. 100 per cent UF_4.

A range of graphite standards were prepared with the impurity elements of interest at different concentrations, together with Y as internal reference standard. The method followed to prepare these graphite standards is given on page 26. The concentration range of these graphite standards is as follows:

UF_4 used: stoichiometric i.e. 75,8% per cent U.

Concentrations: 100 µg X /g UF_4
200 µg X /g UF_4
500 µg X /g UF_4
700 µg X /g UF_4
1 000 µg X /g UF_4

Expressed relative to U, the concentrations $(C_x)_{std}$ for each impurity element X, become:

132 µg X /gU
264 µg X /gU
660 µg X /gU
924 µg X /gU
1 319 µg X /gU

The concentration of Y added to each of the above graphite standards as internal standard is 132 µgY/gU.

These standards were used to quantify the impurity elements in the blank UF_4. Using standard addition methods, each of the above graphite standards was mixed with the blank UF_4 sample in the ratio of one to one by mass. Similar to the blank UF_4 graphite matrix sample, each spiked sample is analysed several times to obtain an instrument signal, $(Q_x/\bar{Q}_y)_{UF_4+std}$, for element X relative to the internal standard, Y. The concentration of each element X can be determined on the basis of equation (9) discussed on page 101:

$$(C_x)_{UF_4} = (C_x)_{std} \cdot \frac{(Q_x/\bar{Q}_y)_{UF_4+std}}{(Q_x/\bar{Q}_y)_{UF_4} - (Q_x/\bar{Q}_y)_{UF_4+std}}$$

Results are given in Table 5.4 as C_x, in μgX/gU.

Table 5.4: Blank UF_4 quantification

Element	Isotope	Isotopic Abundance (%)	Charge State	n	Std Error at 95% CL (%)	C_x (μg X/gU)
Al	27	100	2	8	21,36	5,6
P	31	100	2	5	34,85	76,7
Ca	40 42	96,94 0,65	2 2	9	12,48	25,2
Si	30	3,09	1	5	13,59	77,4
S	32	95,0	1	5	38,74	385,4
Cl	35 37	75,72 24,28	1 1	10	21,35	52,5
Zn	64 67	48,89 27,77	1 1	8	23,78	4,0

The concentration value for S is quite high (385,4 μgS/gU). This greatly influences the calibration line. On the x-axis of the calibration curve, the ratio C_y/C_x is plotted where $C_x = (C_x)_{std} + (C_x)_{UF_4}$. When the background concentration of an element X in the blank UF_4, $(C_x)_{UF_4}$, is large, the ratio C_y/C_x becomes smaller, where C_y is taken as constant. This makes the gradient of the regression line inaccurate and limits the calibration range. The other impurity elements have background concentrations which do not influence the calibration.

The C_x values in Table 5.4 determined for impurity elements in the blank UF_4 are only for the elemental states. The fluorinated species of the elements have not been considered. When analysing UF_4 samples with the spark-source mass spectrometer, it can be assumed that the same degree of fluorination of the elements takes place in the sample as with the UF_4 calibration samples. This assumption is valid if the unknown sample is also stoichiometric UF_4 and the sparking parameters used to generate ions are identical for the UF_4 sample as for the UF_4 calibration samples.

The chemical structures of the impurity elements in the UF_4 sample are assumed to be similar to those in the UF_4 calibration samples. The plasma generated between the two electrodes in the ion source provides the equalising locality for such differences. In this plasma the chemical structures are broken in the process of atomisation and ionisation and recombination of species can take place.

The preparation and characterisation of graphite standards to obtain relative sensitivity factors (RSF's) for impurity elements in a UF_4 sample were done under serious production pressures due to the study of reactions in the uranium fuel production process and time was not allowed to analyse the blank UF_4 sample more comprehensively. It was nevertheless decided to include the results in this thesis as they were reasonable in terms of the precision of the method and made a major contribution to the solving of the production problems at the time. The fact that the UF_4 work was done as an additional project under severe time constraints must be kept in mind when accessing the small number of data points on which the principles have been demonstrated.

The high standard errors at 95 % confidence level (CL) for P (34,85 %) and S (38,74 %) can be ascribed to the small number of data points which were statistically acceptable. This shows how the $(C_x)_{UF_4}$ values for these two elements fluctuated over the concentration range of the standards resulting in the C_x values at higher concentrations being rejected leaving $n = 5$ with still a larger error in the remaining $(C_x)_{UF_4}$ values. The standard error at 95 % CL obtained for Si (13,59 %) with $n = 5$ seems to be the exception where the remaining $(C_x)_{UF_4}$ values show a better standard error at lower concentration levels of the graphite standards. For the above three elements, namely P, Si and S, their concentrations present in the UF_4 sample are the highest, which has a direct influence in the standard errors at 95 % CL.

For the remainder of the impurity elements in the blank UF_4 sample, the standard errors at a 95 % CL show typical values comparable to the precision of the method, namely ~ 20 %. The larger value of n for these elements also shows the reliability of the lower $(C_x)_{UF_4}$ values over the concentration range of the graphite standards.

5.3.2 Calibration curves

The procedure used to construct calibration curves is given in detail on page 137. A few interesting observations are highlighted below.

Similar to procedures followed for the U_3O_8 matrix (see page 109), the instrument signal, $Q_x/Q_{\bar{y}}$, is plotted on the y-axis and the ratio between the concentrations, C_y/C_x, is plotted on the x-axis. The value of C_x in C_y/C_x is taken as the sum of the concentrations of an element X in the prepared graphite standard plus the value of the blank UF_4, expressed as, $C_x = C_{std} + C_{UF_4}$, where C_{UF_4} is obtained from Table 5.4.

The slope of the resultant curve is the relative sensitivity factor (RSF) of that particular impurity element X present in the matrix UF_4 relative to an internal reference standard, Y.

Theoretically, the calibration curve should pass through the origin (see page 139). The values of the intercept on the y-axis, c, listed in Table 5.5 are in accordance with this fact for most of the elements. The values obtained for P and Cl must be kept in perspective as the values of m for these two elements are also large in magnitude compared to the rest. Negative values for c on the y-axis could indicate a minimum detection value for C_x on the x-axis. Below this minimum detection value, non-linearity is evident. For the purpose of this investigation, the highest concentration measured was 1319 µg X/gU. Al and Zn display good linearity over the entire concentration range.

Table 5.5: UF_4 Calibration curve parameters

Element	Isotope	Isotopic Abundance(%)	Charge State	m (RSF)	α (%)	c	r	n
Al	27	100	2	2,0059	0,84	0,0008	0,9999	10
P	31	100	2	25,7454	10,6	-0,9496	0,9917	10
Ca	40 42	96,94 0,65	2 2	0,6104	3,64	-0,0169	0,9980	16
Si	30	3,09	1	0,9438	8,38	-0,0490	0,9948	10
S	32	95,0	1	0,6891	26,9	-0,0123	0,9575	9
Cl	35 37	75,72 24,28	1 1	20,0095	4,82	-0,9232	0,9965	16
Zn	64 67	48,89 27,77	1 1	0,4946	0,87	0,0279	0,9999	10

The calibration graph for Zn in the UF_4 matrix is given in Figure 5.4 as an example of a good calibration curve.

The calibration graph for S in a UF_4 matrix is given in Figure 5.5 as an example of a poor calibration curve.

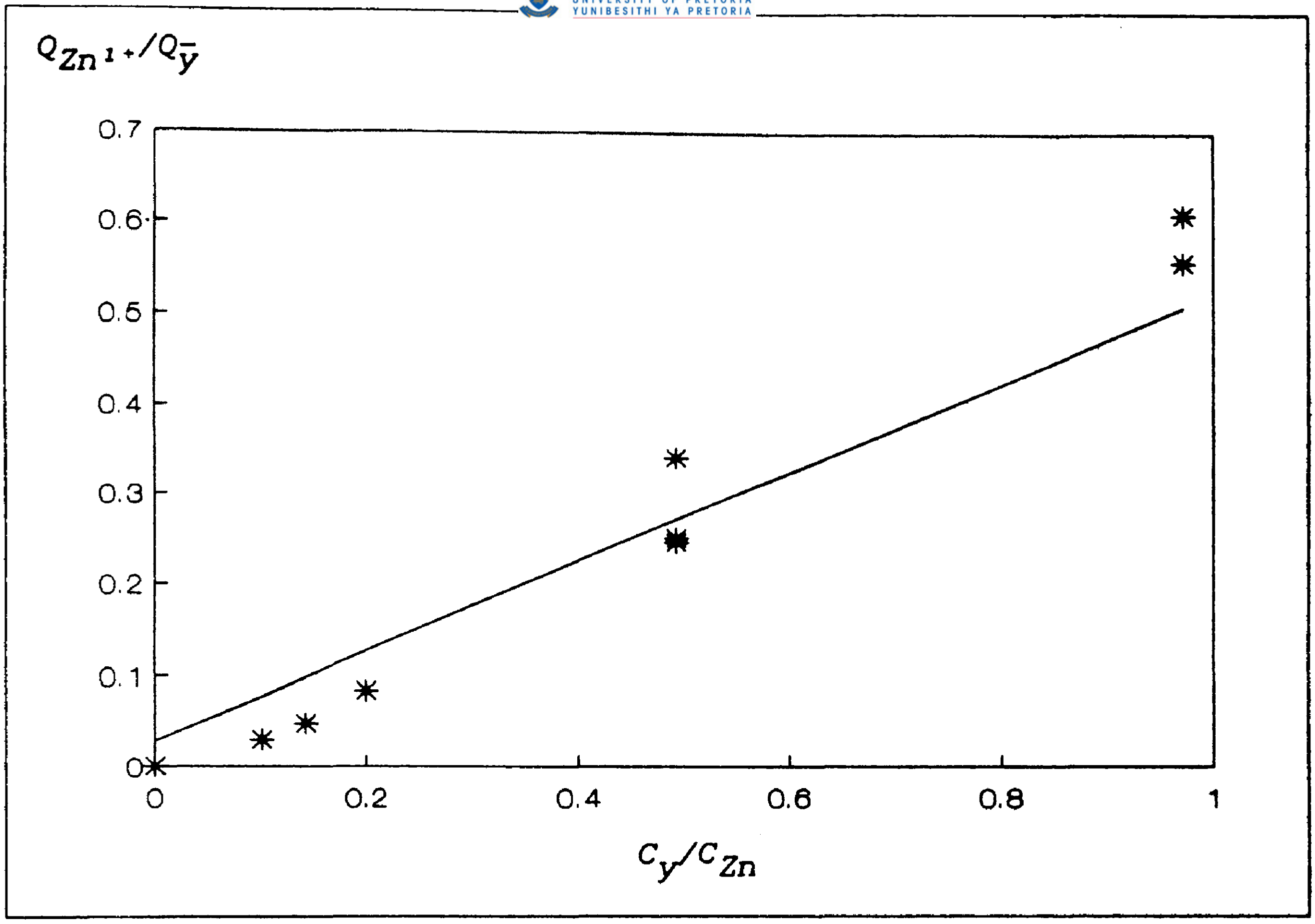


Figure 5.4: *Calibration curve for Zn^{1+} in a UF_4/graphite matrix*

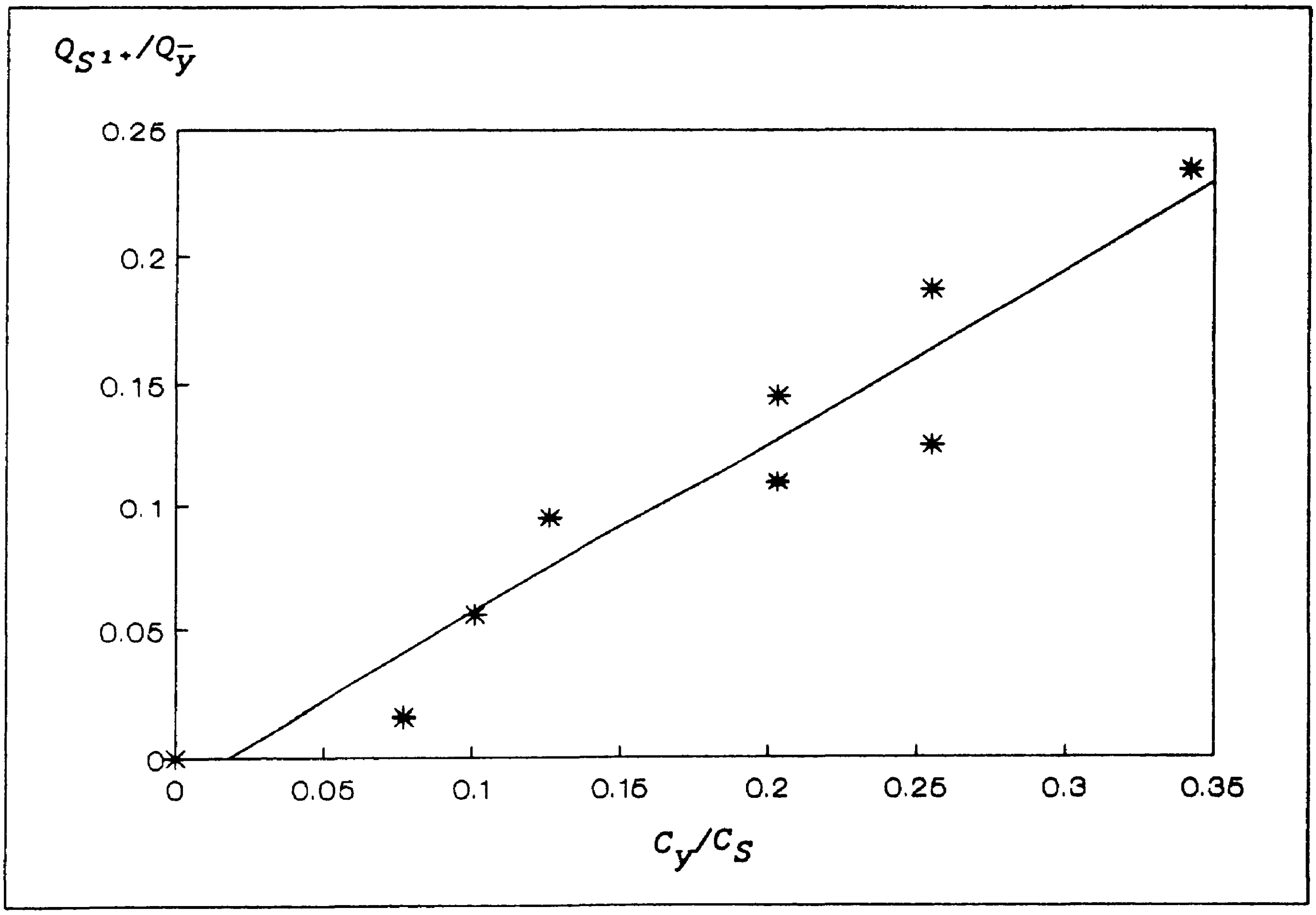


Figure 5.5: *Calibration curve for S^{1+} in UF_4/graphite matrix*

The poor fit of data for S is manifested through the relatively large error in the slope (α = 26,9%) and the high value obtained for S in the blank UF_4. Where blank values are reasonably high, uncertainties in these values are reflected in all other data points. This also happens when standards are added to a quantity which is not known in absolute terms.

The value of n in Table 5.5 is an indication of the number of data points used to construct the calibration curves, where each data point is taken as a single analysis. The value for the blank is also incorporated as a data point.

5.3.3 Relative Sensitivity Factors (RSF's) - UF_4

For the impurity elements investigated in a UF_4 matrix, various physico-chemical properties were studied in order to find a qualitative solution for the very high RSF's obtained for P (25,7454) and Cl (20,0095) listed in Table 5.5. Properties such as first and second ionisation potentials (I_p), bond strength (B_s) of the F-X species, heats of formation (H°_f) of gaseous atoms from elements in their standard states, heat of vaporisation (H°_{vap}), electronegativity (E_{neg}), melting points (M_p) and boiling points (B_p) were studied [28]. No specific physico-chemical property can be singled out to explain anomalies in RSF's as each property plays a role within the plasma. When the melting points and heats of vaporisation are compared between the various elements, it is apparent that P and Cl have the lowest values. However, these elements also have of the highest E_{neg} and ionisation potentials.

5.4 Semi-quantitative analysis

5.4.1 50% Transmission intercept method

This method is more time consuming than the appearance level method (see page 132) but is still quicker than setting up the MD100 microdensitometer to obtain analytical data. Instruments required to perform this method are a Hilger & Watts* microphotometer Model L-500-2 equipped with a carriage to hold a photographic plate and a Fluke# multimeter. Many of the principles and preliminary procedures discussed in detail for the appearance level method also apply to this method. However, only the operational procedure will be discussed below.

The marked photographic plate is positioned and the lens focused, once the light of the photocell has been switched on. A clear plate region of at least 5mm in diameter is made on the photographic plate where there are no spectral lines of interest, by scraping away the emulsion on the photographic plate. This spot will serve as the 100% transmission region in order to calibrate the multimeter.

The intensity of the light is adjusted by means of the photocell amperage so that when the beam of light is mechanically shut off

* Hilger & Watts Ltd, 98 St Pancras Way, Camden Road, London NW1.

John Fluke MFG. Co. INC, P.O. Box 43210, Mountlake Terrace, Everett, Washington, 98043, U.S.A.

there is 0% transmission of light and when the beam of light passes through the clear plate region there is a 100% transmission of light through the photoplate. The Fluke digital multimeter is coupled to the photocell output using its 1 volt scale so that 0% transmission is zero volt on the multimeter and 100% transmission is 1,0 volt on the multimeter. The second decimal scale is sufficient for this method as a reading of 0,65 volt on the multimeter gives a reading of 65% transmission of light through the spectral line. Dark spectral lines on the photoplate will have lower percentage transmission of light through them than lighter spectral lines. The 50 % transmission intercept method can now be implemented.

An element of known concentration is used to obtain a k-factor e.g. U or Y. The $^{234}U^{2+}$ spectral line at m/e 117 is used as internal standard or the $^{89}Y^{1+}$ or $^{89}Y^{2+}$ spectral lines at m/e 89 and 44,5, respectively, can be used as internal standard if Y is present in the sample. A transmission curve is obtained by plotting on the y-axis, using ordinary graph paper, the multimeter reading multiplied by 100 to obtain a percentage transmission for each spectral line on the photographic plate. This is plotted against the natural logarithm on the x-axis of the applicable exposure value of each spectral line on the photographic plate i.e. % T on the y-axis and ln Q on the x-axis. From this transmission curve, the exposure value at 50 % transmission is read off the graph paper and is used in the general formula to obtain a k-factor.

The same procedure is followed as above to obtain a transmission curve for an element X of interest. The exposure value at 50 % transmission is used, together with the k-factor obtained from the internal reference to obtain the concentration value, C_x, of element X. However, this concentration is only for that particular isotope of element X. In order to obtain the total concentration C_x of element in the sample, the isotopic abundance of the applicable isotope measured must be incorporated.

This method is suitable to obtain concentration values for impurity elements in a sample where no relative sensitivity factors are available. In this case the RSF is taken as unity and the final result obtained differs from the true value by about a factor of two or three. The fact that no background correction has been incorporated must be borne in mind. This method can be utilised with high and low concentrations of impurity elements as long as there is a spectral line that can produce a workable transmission curve. Both the semi-quantitative methods are extremely useful for analysing uranium samples where no standard is available. In this case the uranium is taken as the internal standard and used to quantify impurity elements.

5.4.2 Appearance level method

This method is the more reliable method of the two used for semi-quantitative analysis. However, its interpretation differs from analyst to analyst as will be illustrated below. The only instrument required to perform this method is a microscope which is equipped with a carriage to hold a photographic plate. Whilst looking through the eye-piece of the microscope, the analyst must be able to move the carriage holding the photographic plate, along both the x- and y-axes. The x-direction gives the analyst the opportunity to view the spectrum on the photographic plate in its entirety whereas movement in the y-direction focuses on a specific area of the photoplate and the number of different exposures in the form of spectral lines can be counted. This last step is the essence of the method.

If an uranium oxide sample, for example U_3O_8, has been mixed with graphite powder spiked with the internal reference standard, Y, of known concentration, then the U and/or Y are used as the elements of known concentration. A prerequisite for using the U line as reference, is that the isotopic composition is known. If the U is natural, then the concentrations of the various isotopes are known and can be used as reference concentrations. This is shown below as an example.

Uranium used: natural

isotopic abundance (converted to mass percent): 238 = 99,286
235 = 0,710
234 = 0,0055

thus concentration of: ^{238}U = 992 860 µg $^{238}U/g\ U_3O_8$
^{235}U = 7 100 µg $^{235}U/g\ U_3O_8$
^{234}U = 55 µg $^{234}U/g\ U_3O_8$

The concentration of the ^{234}U isotope of uranium is normally used as it has a value similar to impurity levels in the U_3O_8.

The above concentrations can be expressed in general ppm terms as µg of the U isotope per total mass of U (in grams). For natural uranium in U_3O_8 the concentrations are:

^{238}U = 882 425 ppm
^{235}U = 6 167 ppm
^{234}U = 47,8 ppm

When graphite powder spiked with a known concentration of Y is mixed with the U_3O_8, it is done in the ratio of five parts U_3O_8 to one part graphite by mass. This was shown on page 30. The concentration of the Y in the graphite is typically 80 µg Y/gC. When mixed with U_3O_8, the concentration of Y relative to uranium is approximately 20 µg Y/gU. These two concentrations are used when applying the appearance level method.

When a set of spectral lines belonging to a specific element on the photographic plate is investigated under the microscope, dark lines at longer exposures up to light lines at shorter exposures, are observed. At very short exposures, no spectral lines are detected depending on the concentration level of that element in the sample.

The faintest detectable spectral line is called the appearance line. According to the exposure pattern used, this appearance line thus has a specific appearance exposure. The appearance exposure can thus be defined as that exposure necessary for a specific impurity element present at a certain concentration level to become visible to the analyst. This is where the difference in interpretation of the appearance level method varies from analyst to analyst. What might be the appearance exposure for one analyst is not necessarily that for the other analyst.

When performing semi-quantitative analyses with this method, both the Y^{1+} and Y^{2+} lines at masses 89 and 44,5, respectively, are scrutinized to obtain appearance exposures. Similar to quantitative analysis procedures, the mean of these two values is obtained:

$$Q_{\bar{y}} = \frac{Q_{y^{1+}} + Q_{y^{2+}}}{2}$$

When applying the general formula for spark-source mass spectrometry,

$$\text{concentration (C)} = \frac{\text{k-factor}}{\text{exposure (Q)}}, \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

the k-factor for Y , K_y, can be obtained:

$$K_y = C_y . Q_{\bar{y}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

where:

C_y is the concentration of the internal standard Y, relative to the U content, i.e. typically 20 μg Y/gU in the above example, and

$Q_{\bar{y}}$ is the mean appearance exposure of the internal standard.

For an unknown impurity element X present in the U_3O_8 sample, the appearance exposure, Q_x, is determined using the same method as described above.

Using the above Q_x and K_y from equation (2) in equation (1), the concentration C_x of element X relative to the internal standard is determined:

$$C_x = \frac{K_y}{Q_x} \qquad \ldots\ldots\ldots\ldots\ldots \quad (3)$$

If the internal standard is not present, the U spectral lines are used in exactly the same way. However, only the $^{234}U^{2+}$ spectral line at m/e 117 is suitable for use. The concentration of an element X is then expressed relative to the ^{234}U isotope.

This method is a quick way to obtain a concentration for an element without using relative sensitivity factors. The result can differ by a factor of two or three compared to the use of relative sensitivity factors (RSF's). In the above case, the sensitivity of an element X relative to an internal standard is taken as unity. If a RSF does exist for an element X relative to Y in a specific matrix, then it can be used together with the usual formula given below which was derived on page 98:

$$C_x = \frac{RSF \,.\, C_y}{\frac{Q_x}{\bar{Q}_y}} \qquad \ldots\ldots\ldots\ldots\ldots \quad (4)$$

The appearance exposure of element X, Q_x, is expressed as a ratio together with the mean appearance exposure of the internal standard, $\bar{Q}_y$. The concentration C_x obtained for element X is only the concentration of that particular isotope of element X. In order to obtain the total concentration of the element, the concentration obtained for that particular isotope measured, is divided by its isotopic abundance and multiplied by 100 to cancel the percentage.

CHAPTER SIX

EVALUATION OF THE METHOD

6.1 *Statistical significance of results*

6.1.1 *Statistical approach*

Data interpretation is based on the graphic method [29, 30]. This incorporates the use of calibration lines which are obtained from plotting the instrument signal, y, against the concentration, x, of an element. The relationship between x and y can be derived by linear regression using the standard formula:

$$y = mx + c \qquad \dots\dots\dots\dots\dots \quad (1)$$

where:

m is the slope of the calibration line, and

c is the intercept of the y-axis.

The general spark-source mass spectrometry formula [8] can be interpreted on this basis:

$$C_x = \frac{K_x}{Q_x} \qquad \dots\dots\dots\dots\dots \quad (2)$$

where:

C_x *is the concentration of element X,*

K_x *is a constant and*

Q_x *is the exposure value at 50% transmission of element X.*

Equation (2) can be rewritten in the form of equation (1) as follows:

$$\frac{1}{Q_x} = K_x \cdot C_x$$

The intercept c, on the y-axis of equation (1) is taken as zero and is explained later on in this section (see page 139).

The same general formula applies for the internal standard Y, namely:

$$C_y = \frac{K_y}{\bar{Q}_y} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$

$\bar{Q}_y$ is the mean exposure value of Y for the charge states 1+ and 2+ (see page 29).

Combining equations (2) and (3) gives:

$$\frac{Q_x}{\bar{Q}_y} = \frac{K_x}{K_y} \cdot \frac{C_y}{C_x} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

where:

$\frac{Q_x}{\bar{Q}_y}$ is the instrument signal, expressed as the ratio between the exposure value, Q_x, of element X at 50% transmission and the exposure value $\bar{Q}_y$, of the internal reference standard, Y, at 50% transmission;

$\frac{C_y}{C_x}$ is the ratio between the concentration of the internal reference standard, Y, and the concentration of element X which is given in µg X/gU; and

$\frac{K_x}{K_y}$ is the slope, expressed as the relative sensitivity factor (RSF) [18, 31] of an element X, relative to the internal reference standard, Y.

The concentration of the internal standard, Y, is taken as 20 µg Y/gU when analysing unknown U_3O_8 samples and 132 µg Y/gU when analysing unknown UF_4 samples. The choice of these concentrations of the internal standard is comprehensively described on pages 29, 103 and 122.

The concentration of an element X varies according to the range of graphite standards prepared. The choice of these ranges is comprehensively described on page 103 for a U_3O_8/graphite matrix and on page 122 for a UF_4/graphite matrix.

The instrument signal, Q_x/Q^{-}_y, is obtained when doing data interpretation and is taken as the intercept at a 50% transmission of the Hull function plot. This is described on page 36.

The origin (0;0), of the calibration graph is also incorporated in the calibration line. This is shown as follows:
When C_x tends to infinity, then the expression C_y/C_x tends to zero when C_y is taken as constant. From equation (2), when C_x tends to infinity, then Q_x tends to zero. Likewise, the expression Q_x/Q^{-}_y tends to zero when Q^{-}_y is taken as constant because C_y is constant. Thus both expressions tend to the origin (0;0) when C_x tends to infinity. This verifies the use of the origin as a data point when compiling calibration graphs.

Linear regression formulae [29] (see Appendix A on page 174) are used to determine the standard error, s_m, in the slope of the regression line. The confidence limits of the slope, expressed as α, is given by the following formula [32]:

$$\alpha = s_m \cdot t \qquad \ldots\ldots\ldots\ldots\ldots \quad (5)$$

where:
s_m is the standard error of the slope, and
t is the Student's t-value [33] at a 95% confidence level (CL) with (n-2) degrees of freedom where n is the number of data points (x;y) used to draw up the calibration graph.

The parameters RSF, α,c, r and n obtained from the regression line are given in Table 5.2 (see page 111).

6.1.2 Propagation-of-errors approach [30, 34]

This method is used when determining the concentration C_x, of an element X, in an unknown U_3O_8 sample. Equation (4) can be rewritten as follows:

$$C_x = \frac{(RSF \pm \alpha)\ .(C_y \pm c_y)}{\frac{Q_x}{\bar{Q}_y} \pm 2s} \quad (95\%\ CL) \ \ldots\ldots\ldots\ldots \quad (6)$$

The confidence limits α, of the slope or relative sensitivity factor is obtained from Table 5.2 on page 111. Likewise, the applicable relative sensitivity factor RSF, is given in Table 5.3 (see page 120). The concentration of the internal standard, Y, given by C_y, is taken as 20 µg Y/gU where graphite powder has been spiked with 80 µg Y/gC. This graphite powder, called UFY80, is used as electrode material when analysing unknown U_3O_8 samples. The error in C_y, given by c_y, is taken as 0,5% which is the maximum imprecision of a 1 000 µl varipette used to dispense the Y ICP standard solution. The precision of the Mettler H10T mass balance used to weigh out the required mass of graphite powder is 0,1 mg which gives an error of 0,002% when 5 grams of graphite is used. The Y ICP standard solution is certified to <0,01% and the error is not significant. These errors can be ignored statistically and only the error in the varipette, 0,5%, is taken as c_y [38].

The precision of the method is also known and is given in Table 6.1 (see page 147). For a single analysis of an unknown U_3O_8 sample, the error coupled to the instrument signal, $Q_x/\bar{Q}_y$, for element X is taken as twice the standard deviation, 2s [35, 38]. This is based on the assumption of a normal distribution of results where an analysis result has a 95% chance of lying within two standard deviations of the mean.

When considering the general error formulae used in composite errors, the following applies [36, 37]:
For a number of quantities, n, with means $\bar{x}_1$, $\bar{x}_2$, ----, $\bar{x}_n$, with standard errors α_1, α_2, ---, α_n, the standard error of

any function of $\bar{x}_1$, $\bar{x}_2$, ---, $\bar{x}_n$, namely, $f(\bar{x}_1, \bar{x}_2, ---, \bar{x}_n)$ is

given by α, where $\alpha^2 = \left(\frac{\partial f}{\partial \bar{x}_1}\right)^2 \alpha_1^2 + \left(\frac{\partial f}{\partial \bar{x}_2}\right)^2 \alpha_2^2 + --- + \left(\frac{\partial f}{\partial \bar{x}_n}\right)^2 \alpha_n^2$

The quotient of two mean values is given by:

$$f(\bar{x}_1, \bar{x}_2) = \frac{\bar{x}_1}{\bar{x}_2}$$

thus $\frac{\partial f}{\partial \bar{x}_1} = \frac{1}{\bar{x}_2}$ and $\frac{\partial f}{\partial \bar{x}_2} = -\frac{\bar{x}_1}{\bar{x}_2}$

$$\text{This gives } \alpha^2 = \left(\frac{1}{\bar{x}_2}\right)^2 \alpha_1^2 + \left(-\frac{\bar{x}_1}{\bar{x}_2}\right)^2 \alpha_2^2$$

$$= \frac{1}{\bar{x}_2^4} \left(\bar{x}_2^2\alpha_1^2 + \bar{x}_1^2\alpha_2^2\right)$$

$$\text{Therefore} \quad \alpha = \frac{1}{\bar{x}_2^2} \sqrt{\bar{x}_2^2\alpha_1^2 + \bar{x}_1^2\alpha_2^2} \quad \ldots\ldots\ldots\ldots\ldots \quad (7)$$

The product of two mean values is given by:

$$f(\bar{x}_1, \bar{x}_2) = \bar{x}_1 . \bar{x}_2$$

$$\text{thus } \frac{\partial f}{\partial \bar{x}_1} = \bar{x}_2 \quad \text{and} \quad \frac{\partial f}{\partial \bar{x}_2} = \bar{x}_1$$

$$\text{This gives } \alpha^2 = \bar{x}_2^2 \, \alpha_1^2 + \bar{x}_1^2 \, \alpha_2^2$$

$$\text{and} \qquad \alpha = \sqrt{\bar{x}_2^2 \, \alpha_1^2 + \bar{x}_1^2 \, \alpha_2^2} \qquad \ldots\ldots\ldots\ldots\ldots \; (8)$$

Applying the above equations (7) and (8) to equation (6), the standard error, s_{C_x}*, of the concentration of element X in the unknown sample is derived.*

$$\text{Thus } s_{C_x} = \frac{1}{(\frac{Q_x}{Q_y})^2} . \sqrt{(\frac{Q_x}{Q_y})^2 . (C_y^2 \alpha^2 + RSF^2 c_y^2) + (RSF.C_y)^2 . (2s)^2} \quad \ldots\ldots \; (9)$$

The final result of element X is reported as:

$$C_x \pm s_{C_x} \quad (95 \text{ \% CL})$$

This gives the confidence interval derived using the propagation-of-errors method at a 95 % confidence level.

6.1.3 Precision

In order to determine the precision coupled to the analysis of U_3O_8/graphite matrix samples using spark-source mass spectrometry, three of the prepared graphite standards with concentrations of 1,0; 10,0 and 50,0 μg X /gU were each analysed six times (i.e. n = 6) mixed with the base U_3O_8 (see page 103). The results obtained are tabulated in Table 6.1 on page 147. The precision that is obtained is for both the instrument and the analyst.

The standard error at a 95% confidence level (CL) was determined using the following formula [37]:

$$\bar{x} \pm \frac{t.s}{\sqrt{n}} \text{ at } 95\% \text{ CL} \qquad \ldots\ldots\ldots\ldots\ldots \ (1)$$

where:

$\bar{x}$ is the mean of the six analyses of one standard;
s is the standard deviation of the six analyses; and
t is the Student's t-value taken at a 95% confidence level using (n - 1) degrees of freedom (ν).

Before the above formula could be used, the data obtained had to be subjected to the Dixon outlier test [38, 39, 40, 41] in order to ascertain whether there were any "mavericks". The Dixon outlier test assumes that the parent population from which the measurements are obtained is normally distributed.

One way of assessing a suspect measurement is to compare the difference between it and the measurement nearest to it in size with the difference between the highest and lowest measurements. The ratio of the differences is known as Dixon's Q and is given as Q_{calc} in the following basic formula:

$$Q_{calc} = \frac{|\text{ suspect value - nearest value }|}{(\text{largest value - smallest value})} \qquad \ldots\ldots \ (2)$$

The critical values of Q, given as Q_{tab}, are taken from the table of critical values for Q at a 95% confidence level (CL).

The following reasoning is applied in the Dixon test:
If $Q_{tab} \geqslant Q_{calc}$, then the suspect value is retained;
if $Q_{calc} > Q_{tab}$, then the suspect value is rejected.
From the table of critical values of Q, the sample size in this case is taken as six.

It is important to note that at a 95% CL there is still a 5% chance of incorrectly rejecting the suspect value. When measurements are repeated only a few times rejection of one value makes a great difference to the mean and standard error. This has a considerable effect on the estimation of the precision. The importance of caution in rejecting outliers cannot be over-emphasised. There is also the possibility of two suspect values which leads to masking in the application of the Dixon Q-test.

Using the above approach, suspect values were rejected for a number of elements from each of the standards. This is shown in Table 6.1 where n = 5. For Mo^{1+} (n = 4) and Sm^{1+} (n = 3), the experimental data obtained was limited as the spectral lines on the photographic plate could not be measured in all the cases.

An assessment of the results tabulated in Table 6.1 reveals that most of the standard errors at a 95% CL are below 20% with the exception of a few cases which will be explained below. This is in accordance with values reported by many other authors [31] who have used electrical detection, radio frequency (RF), glow discharge (GD) and other types of spark-source mass spectrometers for analysing U samples.

The first few elements in Table 6.1, namely B, Mg and Al, have high standard errors at all the concentration levels. This is ascribed to interference of their spectral lines at masses 10 and 11 for B, 12,5 for Mg and 13,5 for Al, due to the spectral lines of the matrix component C at masses 12 and 13. The C spectral lines, being from the major constituent of the sample, are intense and dispersed in the region surrounding them, thus affecting the adjacent spectral lines and their precision, irrespective of concentration.

The standard errors for most of the elements at a concentration level of 1 µg X /gU are relatively high. This is a result of unreliable data obtained from the transmission curves. Only a few points could be utilised in the Hull function plot as most of these were light points. This could also be ascribed to the fact that at this concentration level, the detection limit for some of the elements is reached. Typical examples affected in this manner are Mn^{1+}, Zn^{1+}, Zr^{1+} and the heavier elements such as the rare earths Sm, Eu and Dy.

The high standard errors at a 95% CL for the heavier elements, such as the rare earths at a concentration level of 1 µg X /gU, is ascribed to the fact that these elements provide small ion yields of the various charge states resulting in poor transmission curves. The atomic size of these elements affects the number of ions entering the ion source due to collisions. These ions also have a smaller velocity down the flight tube of the mass spectrometer. All these factors have a decisive impact on the nett total of ions yielded at the photographic plate.

The very high standard error for Mo^{1+} at a 95% CL, namely 84,1%, can be ascribed to the previous reasons (poor ion yield, near the low concentration detection limit, as well as the small number of useful data points). When applying the formula to determine the standard error at a 95% CL, the degrees of freedom (ν) is given as ($n - 1$), i.e. 3 where $n = 4$, which is relatively small. This means that the standard deviation, s, is multiplied by a factor 1,59 (3,182/2) giving a higher standard error. As n gets larger, the factor of $t/\sqrt{n}$ gets smaller, thus reducing the standard error in a significant way.

The standard errors for Ca^{2+} and Si^{1+} are relatively high as the Ca^{2+} spectral line was measured as a doublet and the Si^{1+} spectral line was measured as a triplet. The analyst has to set windows around these lines and this affects the background surrounding the spectral lines which are under scrutiny. This leads to a weaker precision at all concentration levels.

The high standard error for Ni^{1+} at 95% CL at a concentration of 50 µg Ni /gU, namely 34,2%, is verified as follows. From the raw data obtained, there is one data point out of the set of six ($n = 6$) that appears to differ from the remainder. However, when applying the Dixon outlier test to this data point, the test shows that this data point cannot be taken as an outlier and must thus be retained. This leads to the high standard error. If the Dixon outlier test had shown that this point could be rejected, the precision would have been 15,9% for the remainder of the data points ($n = 5$). This could be interpreted as a possible limitation of the Dixon outlier test.

The precision values obtained are used together with the relative sensitivity factors (RSF's) when analysing the unknown U_3O_8 samples where the error in the instrument signal is taken as twice the standard deviation.

TABLE 6.1: Precision for U_3O_8

Element	Charge State	C_x = 1µg X /gU		C_x = 10µg X /gU		C_x = 50µg X /gU	
		Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n
B	1	27,6	6	24,8	6	36,1	6
Mg	2			10,3	5	40,4	6
Al	2			24,7	6	22,6	6
Si	2	38,6	6	11,1	6	16,6	6
Si	1			25,3	6	35,5	6
Ca	2	12,0	6	24,8	6	29,5	6
Ti	2			6,1	5	13,2	6
Ti	1	21,2	6				
V	2			13,9	6	15,9	6
V	1	7,6	6	10,5	6	8,8	6
Cr	2			10,8	6	10,7	6
Cr	1	17,7	6	14,0	6	18,6	6
Mn	2			16,3	6	22,0	6
Mn	1	29,7	6	19,1	6	19,1	6
Fe	2			19,0	6	12,8	6
Fe	1	18,9	6	15,5	6	15,4	6
Co	2			11,2	6	17,2	6
Co	1	6,6	6	5,0	6	17,7	6
Ni	1	19,3	6	2,6	6	34,2	6
Cu	2			7,1	6	17,0	6
Cu	1	15,3	6	15,3	6	19,3	6
Zn	1	32,5	6	8,8	6	21,6	6
Sr	2			10,2	6	17,2	6
Sr	1	18,1	6	9,4	6	15,7	6
Zr	2			8,4	6	15,8	6
Zr	1	36,1	6	6,2	6	11,2	6
Nb	2			10,6	6	15,6	6
Nb	1	18,2	6	10,9	6	5,8	5

Table 6.1: Continued

Element	Charge State	C_x = 1μg X /gU		C_x = 10μg X /gU		C_x = 50μg X /gU	
		Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n	Std Error at 95% CL (%)	n
Mo	2			8,6	6	16,2	6
Mo	1	84,1	4	7,1	6	11,2	6
Ru	2			13,9	6	12,2	6
Ru	1			7,7	5	5,0	5
Cd	1			10,4	6	15,3	6
In	1	23,9	6	11,7	6	21,9	6
Sb	2			7,6	6	8,6	6
Sb	1	34,1	6	12,2	6	16,3	6
Ba	2			8,6	6	8,9	6
Ba	1	27,5	6	15,9	6	17,1	6
Sm	2	48,3	5	9,4	6	10,7	6
Sm	1			18,8	3	17,0	6
Eu	2	33,3	6	7,3	6	14,2	6
Eu	1			5,8	6	8,8	5
Gd	2			6,8	5	9,3	6
Gd	1			8,4	5	5,0	5
Dy	2	32,0	5	14,9	6	9,8	6
Dy	1			7,3	5	12,4	6
Bi	2			25,2	6	15,0	6
Th	2	25,8	6	12,9	6	20,2	6

6.1.4 Confidence Intervals - U_3O_8

Confidence limits of the slope, expressed as α, have a significant influence on the relative sensitivity factor (RSF) derived as the slope of the calibration curve. Large α values mean large uncertainties in the RSF's. These uncertainties must be included in the overall errors calculated for the final analysis results. Values of α greater than 20% in Table 5.2 (see page 111) can be ascribed to a number of reasons, of which the important ones are given below.

The value of n has a significant influence on the value of α. This can be demonstrated using equation (5) on page 139 where the t-value is obtained using (n - 2) degrees of freedom at a 95% confidence level (CL). For n = 7, the t-value from the Students t-Distribution Table is 2,571. The standard error in the slope, s_m, must be multiplied by this number in order to obtain the α value and leads to large confidence limits of the slope.

When determining the calibration curve parameters, each analysis of a graphite standard sample was treated as an individual analysis. Thus, when a graphite standard was analysed in triplicate, the value of n was taken as three. This was typically done using the check graphite standards where some elements were analysed for the first time, e.g. Na, P, K and W. Using two such check graphite standards together with the origin (0;0) gives a t-value of 2,571, where n = 7. This means that a standard error in the slope of 20% becomes a confidence limit of 51,4%. A number of elements in Table 5.2 fall into this category, namely Na^{1+} (11%), P^{1+} (8,1%), P^{2+} (13,6%), K^{2+} (7,8%) and W^{2+} (14,5%), where the standard error is given in brackets after each element.

The ion yields of certain elements with specific charge states at their lowest concentration levels are not very good, with the result that poor transmission curves are obtained. Only a few long exposure values are used in the Hull function plot and the rest of the data points are discarded as light points. The charge state differs from element to element depending on the atomisation and ionisation of the particular element. This can be illustrated when plotting characteristic curves of number of ions yielded against charge state. A number of cases in Table 5.2 where α is near or greater that 20 % can be placed into this category, namely K^{2+}, Ru^{2+}, Ba^{1+}, W^{1+}, Sm^{1+}, Mo^{1+} and Sb^{1+}.

Elements with large atomic radii are more prone to collisions and also have a slower velocity down the flight tube. This leads to fewer ions reaching the photoplate. From Table 5.2, elements falling into this category are Sm^{1+}, W^{2+}, Ba^{1+}, Mo^{1+}, Sb^{1+} and Ru^{2+}.

The correlation coefficient, r, in Table 5.2 can also be coupled to a larger α value. Ideally r should be unity, thus values of $r < 0,90$ show that the fit of calibration data to the regression line is seriously affected by a few bad data points. The inclusion of these bad data points is confirmed by applying the Dixon outlier test which shows that these values have to be retained. However, great caution should be exercised in drawing conclusions from the result of repeated applications of the Dixon's test. If a few statistical outliers are found at a certain particular concentration level this is not very serious, but if several outliers occur at different concentration levels, this may be considered as indicating that the regression line and thus the RSF is inaccurate. This would lead to a large spread of data points resulting in a large standard error in the slope, s_m.

Correspondingly, a larger α value is obtained. Elements in Table 5.2 having poor correlations where r <0,90 are Fe^{1+} (r = 0,853) and Ba^{1+} (r = 0,897). This is in spite of n being large for Fe^{1+} (n = 30) and Ba^{1+} (n = 22). Elements in Table 5.2 having correlation coefficients of r <0,95 are the following: Mg^{2+}, Si^{2+}, Ca^{2+}, Mo^{1+}, Sb^{1+} and Sm^{1+}.

For Mg^{2+}, Si^{2+}, Fe^{1+} and Na^{1+} it is significant to note that these elements all have high background concentrations in the blank base U_3O_8 sample. The influence of this high blank concentration on the calibration line is discussed on page 105. This effectively reduces the range on the x-axis of the calibration plot. Typically, for Fe^{1+} the range on the x-axis is from zero to 0,2844. The spread of data points in this case is larger than over a greater range on the x-axis and results in a poor fit of the data points on the regression line. Another reason for Mg^{2+} having an α of 19,3% is the fact that it is measured at m/e 12,5 which lies inbetween the two spectral lines of the major component of the U_3O_8/graphite mixture, namely ^{12}C and ^{13}C at m/e 12 and 13, respectively. Intense fogging on the surrounding background makes the measurements of Mg^{2+} difficult and inaccurate.

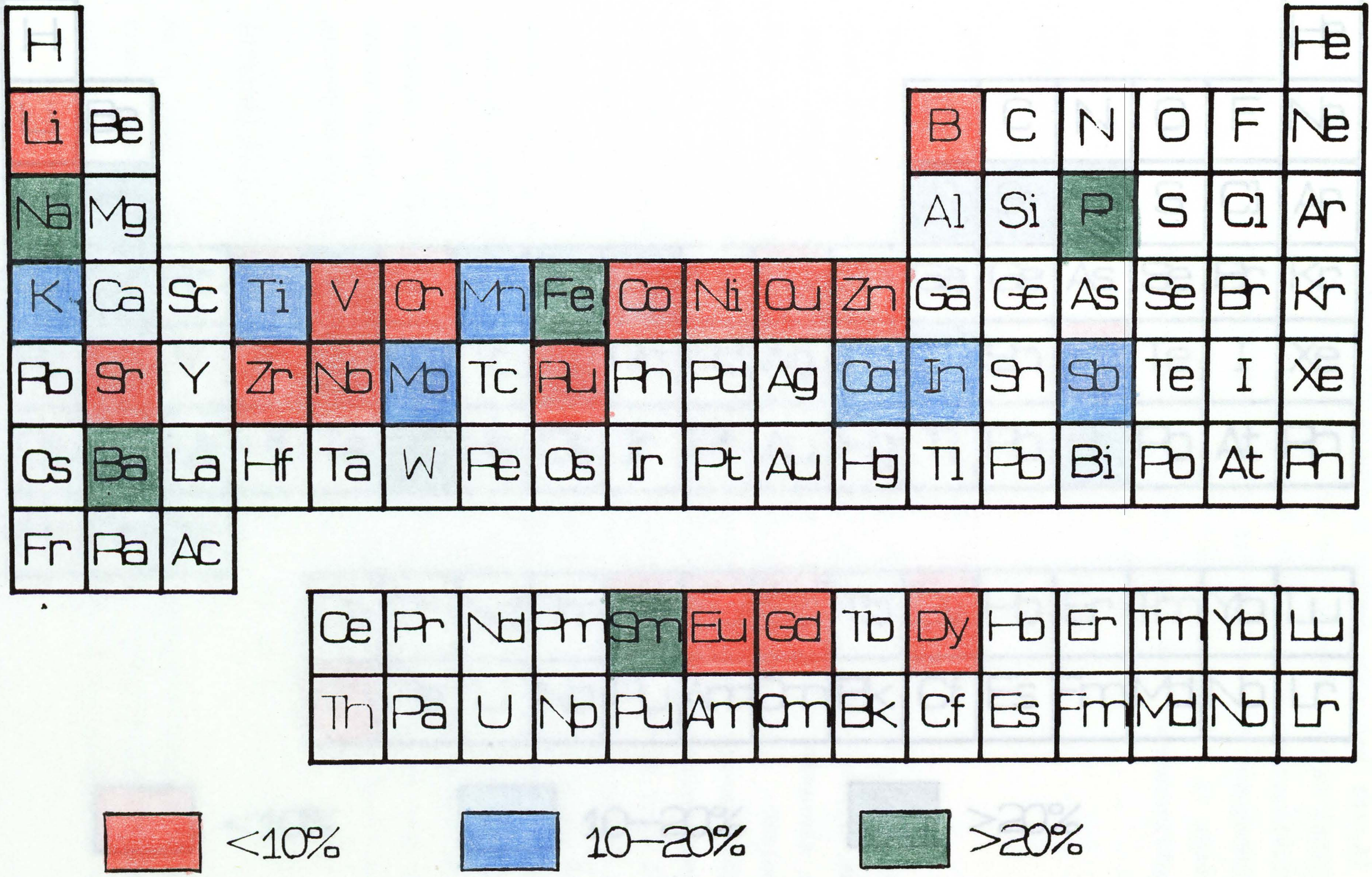
When using α values to determine the error coupled to an element's concentration in an unknown U_3O_8 sample, the analyst must exercise great care. In the case of Ba^{1+} (23,0%) and Sm^{1+} (45,0%), the analyst should avoid using these charge states, and should rather use the other charge states where the α values are more acceptable. The same argument applies for W^{2+} (40,3%).

The α value for the impurity elements in a U_3O_8/graphite matrix are tabulated in Table 5.2. However, these have also been given as a visual presentation in the form of two periodic tables, the first for the singly charged species, Figure 6.1, and the other for the doubly charged species, Figure 6.2. It is demonstrated that the appropriate application of the guidelines for quantification enables the acquisition of analytical data within very acceptable confidence intervals for most of the selected elements.

6.1.5 Confidence Intervals - UF_4

The confidence limits of the slope, expressed as α and as a percentage in Table 5.5 on page 127, is a direct measure of the uncertainty coupled to the RSF. The α value for S is the only one which is relatively high (26,9%) for impurities in a UF_4 matrix. This could be attributed to a number of factors of which the most important is the fact that sulphur is measured at mass 32 as a doublet with the main interference being $^{64}Zn^{2+}$. This could influence the data and result in a bigger spread of data points for the calibration curve. This bigger spread implies a larger standard error in the slope, resulting in a large α value. This fact is also supported by the relatively poor correlation coefficient obtained ($r = 0,9575$) for the regression line.

The α value for S could also be influenced by the relatively high background concentration in the blank UF_4 ($C_x = 385,4$ µgS/gU). This value is used together with the concentration of the standard to define the x-value in a data point (x;y) when applying linear regression. The higher the blank concentration, the more influence it has on the C_y/C_x value on the x-axis. The standard error for S in the blank UF_4 at a 95% confidence level (38,74%) is also an indication of the difficulty experienced to obtain reliable data for sulphur in a UF_4 matrix.



H																	He
🟥 Li	Be											🟥 B	C	N	O	F	Ne
🟩 Na	Mg											Al	Si	🟩 P	S	Cl	Ar
🟦 K	Ca	Sc	🟦 Ti	🟥 V	🟥 Cr	🟦 Mn	🟩 Fe	🟥 Co	🟥 Ni	🟥 Cu	🟥 Zn	Ga	Ge	As	Se	Br	Kr
Rb	🟥 Sr	Y	🟥 Zr	🟥 Nb	🟦 Mo	Tc	🟥 Ru	Rh	Pd	Ag	🟦 Cd	🟦 In	Sn	🟦 Sb	Te	I	Xe
Cs	🟩 Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	🟩 Sm	🟥 Eu	🟥 Gd	Tb	🟥 Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

🟥 <10%

🟦 10–20%

🟩 >20%

<u>Figure 6.1</u>: Confidence intervals (α) at 95% CL for X^{1+} in U_3O_8

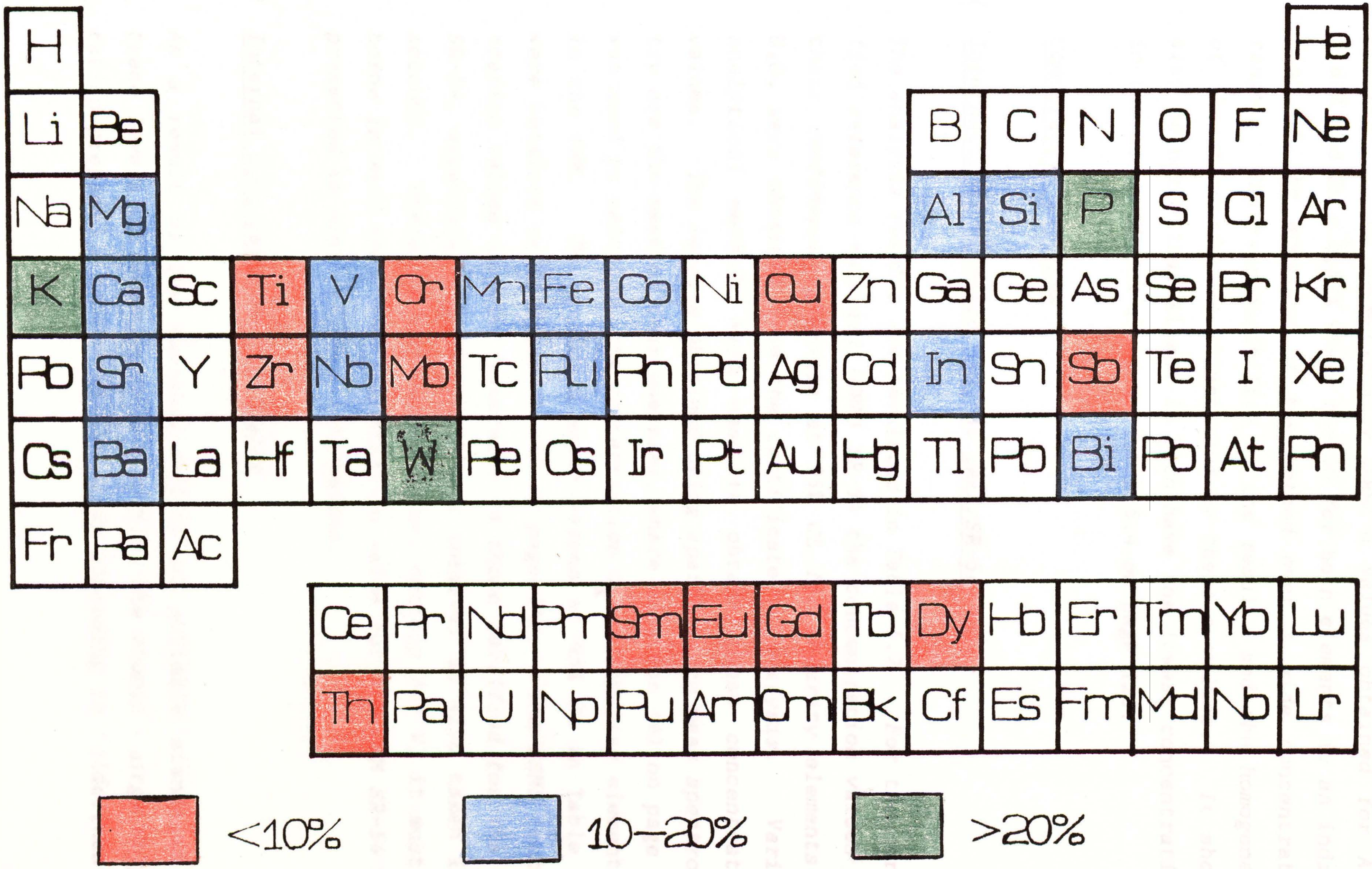


Figure 6.2: Confidence intervals (α) at 95% CL for X^{3+} in U_3O_8

The other α values in Table 5.5 are all acceptable in the sense that they fall within the precision of the instrument and the analyst. The exceptionally good α values obtained for Al = 0,84% and Zn = 0,87% where n = 10 for both elements is an indication of the accuracy of the method over a wide concentration range. The reproducibility of the results and the homogeneity of the standards are illustrated by these α values. It should also be noted that Al and Zn both have the lowest concentrations in the blank UF_4 as shown in Table 5.4 on page 123.

6.2 Comparative analyses

6.2.1 International standard U_3O_8 No IAEA/SR-54

The analysis results are tabulated in Table 6.2. For the certified reference material (CRM) SR-54 the concentration values and their confidence intervals at 95% CL for impurity elements in U_3O_8 were obtained from the certificate of analysis. Various analytical methods were used to obtain these concentration values. The results obtained using spark-source mass spectrometry are the mean of four analyses, where equation (4) on page 136 was used to calculate the concentration C_X of impurity element X in the CRM. The standard error values at 95% CL in Table 6.2 were obtained using equation (9) on page 142. The SSMS concentration values compare favourably to those certified for the CRM SR-54, especially if the confidence interval is also taken into account. Where differences do occur, notibly for V, it must be borne in mind that the concentration value for the CRM SR-54 was presented as non-certified information.

6.2.2 Internal U_3O_8 certified standards

As a result of the non-availability of suitable standards at trace levels of elements in a U matrix, the Atomic Energy Corporation prepared a series of standards according to guidelines as

TABLE 6.2: Comparison of U_3O_8 CRM SR-54 with SSMS

Element	Certified conc. value (µg X /gU)	Confidence interval at 95% CL	SSMS conc. value (µg X /gU)	Std error at 95% CL
Al	71,3	54,8 - 82,0	70,4	15,9
Co	4,2	4,0 - 4,3	5,2	1,3
Cr	3,6	3,1 - 4,3	2,9	0,8
Cu	5,0	4,2 - 6,7	5,7	0,5
Fe	64,7	46,0 - 77,5	66,2	10,2
K	1,7*	-	3,3	0,7
Mg	0,99*	0,81 - 1,1	1,9	0,8
Mn	15,6	14,3 - 16,9	18,4	3,7
Mo	13,0	9,5 - 17,5	12,7	1,1
Na	2,8*	-	3,9	0,8
Ni	11,4	8,4 - 13,9	10,8	2,0
Si	34,3*	18,0 - 53,5	29,8	7,5
Ti	0,98*	-	1,74	0,37
V	3,7*	-	0,12	0,01
Zn	2,4*	0,89 - 3,2	2,2	0,2

* These values are not certified, but are presented as non-certified information values.

laid down by the New Brunswick Laboratory#. These standards covered a wide concentration range and were prepared in a U_3O_8

\# U.S. Department of Energy, New Brunswick Laboratory, 9800
S. Cass Avenue, Building 350, Argonne, Illinois, 60439,
U.S.A.

matrix. The standard with the highest concentration level of impurity elements is called ES 1 and the comparison between the certified value and the concentration value obtained with the spark-source mass spectrometer is given in Table 6.3. The standard with the lowest concentration of impurity elements is called ES 5 and the comparison of results obtained is given in Table 6.7. Standards with concentrations falling inbetween ES 1 and ES 5, named ES 2, ES 3 and ES 4, are given in Tables 6.4, 6.5 and 6.6 respectively.

Of every standard in the ES series of standards, three samplings were each analysed in triplicate. This resulted in each ES series of standards being analysed nine times by a specific analytical technique. The spark-source mass spectrometer (SSMS) concentration values given in Table 6.3 to Table 6.7, are the mean concentrations over nine analyses. These concentration values within an ES standard were also subjected to the Dixon outlier test to ascertain whether there were any outliers before each final mean value was reported.

The formula used to calculate the concentration, C_X, of an impurity element X in each of the ES series of standards is given by equation (4) on page 136. However, this concentration value also contains the contribution from that impurity element also found in the graphite which was used to mix with the U_3O_8 ES series of standards. This has been described on page 108. The concentration levels of impurity elements in the graphite were quantified and deducted from the mean concentration values reported for each of the ES series of standards.

Various analytical methods were used by different laboratories in order to certify these internal U_3O_8 standards, amongst others:

- Inductively coupled plasma (ICP) optical emission spectroscopy (OES),
- Ion chromatography (IC),
- Carrier distillation emission spectroscopy (CDES),
- Atomic absorption spectroscopy (AAS), and
- UV - spectroscopy.

It is beyond the scope of this investigation to go into any detail of how the data obtained for the ES series of standards analysed with the above methods, was evaluated. The certified concentration values and confidence intervals at a 95% CL for the various impurity elements across the ES series of standards given in Tables 6.3 to 6.7 were obtained after the evaluation. These certified values were calculated from the experimental data.

The standard error values at a 95% CL in Tables 6.3 to 6.7 were obtained using equation (9) on page 142. However, the term 2s in this equation was replaced by the term $s.t/\sqrt{n}$ as denoted by equation (1) on page 143. This is in accordance with the fact that the $Q_x/Q_{\bar{y}}$ value used in equation (9) is the mean of several (nine) analyses as previously mentioned in this section. The standard error coupled to this mean $Q_x/Q_{\bar{y}}$ value at a 95% CL is thus derived using equation (1) where n is taken as nine and s is the standard deviation over the nine analyses. The other terms used in equation (9) are identical to those used in equation (6) on page 142 and which were comprehensively described. The use of equation (6) was not warranted as multiple analyses were performed and not just a single analysis.

When comparing the results in Tables 6.3 to 6.7, a number of facts should be kept in mind. The certified values must not be accepted as being the absolute values for particular impurity elements in the series of ES standards. A better representation of the results obtained is given in Appendix C on page 191 where graphs have been compiled for all the impurity elements across the concentration range for each of the analytical methods in comparison to the expected concentration values. In this way anomalies can be detected and comparisons drawn between the spark-source mass spectrometry results and the expected concentration values.

Another interesting fact to consider is whether there is a meaningful difference between a certified value of, for example, 0,1 µg Cd/gU and a SSMS value of 0,64 µg Cd/gU, as reported in Table 6.7. Both these values are less than 1 µg Cd/gU and at these trace levels the detection limits of certain analytical instruments have to be considered. The same could be true for Fe in Table 6.4 where the certified value is given as 208 µg Fe/gU and the SSMS value is given as 264 µg Fe/gU. In view of the various confidence intervals for these two values, it is clear that the analyst should not compare exact values with each other but also take cognicance of the confidence limits coupled to a result when assessing such data.

The SSMS concentration value obtained for Ca across the ES series of standards is higher than the certified concentration values. The higher value could possibly be coupled to an incorrect relative sensitivity factor (RSF) for Ca. This can be seen in the graph for Ca in Appendix C where the graph for SSMS (method B) lies above the dotted line which represents the true concentration values. The very high value for Ca obtained for the ES 1 standard with SSMS was also obtained by three other analytical techniques, namely A, C and D. It has not been possible to confirm the reasons for this difference. Ca is a difficult element to determine with spark-source mass spectrometry and the investigation has not been persued for this element.

The SSMS concentration value obtained for Th across the ES series of standards is higher than the certified concentration values reported for ES 1, ES 2 and ES 3, although no confidence intervals were reported for these values. However, the SSMS results compare favourably to the expected values as shown in the graph in Appendix C.

It should be noted from the graphs in Appendix C that the mass spectrometry results in general, compare remarkably well with the expected standard values.

Table 6.3: Comparison of U_3O_8-Standard ES 1 with SSMS

Element	Certified conc value (μg X /gU)	Confidence interval 95 % CL	SSMS conc value (μg X /gU)	Std Error at 95% CL
Al	234	189 - 279	242	43
B	5,7	5,0 - 6,4	4,9	1,0
Bi	14,3	11,6 - 17,0	13,1	3,0
Ca	272	245 - 299	416	110
Cd	5,5	5,0 - 6,1	6,0	1,3
Co	26,6	23,7 - 29,5	28,8	3,5
Cr	125	77 - 174	154	27
Cu	104	84,4 - 124	120	21
Dy	0,56	0,43 - 0,69	0,71	0,24
Eu	0,56	0,44 - 0,68	0,69	0,16
Fe	827	663 - 990	972	191
Gd	0,64	0,41 - 0,87	0,85	0,34
In	6,2	4,4 - 7,9	8,9	1,6
K	536	481 - 591	379	112
Li	11,5	9,31 - 13,7	13,2	3,8
Mg	56,2	48,5 - 63,9	49,8	14,6
Mn	55,3	47,5 - 63,2	65,1	15,5
Mo	54,6	46,1 - 63,1	59,4	7,3
Ni	233	209 - 259	243	47
Sb	11,2	9,2 - 13,1	13,8	2,8
Si	206	169 - 244	221	65
Sm	0,60	0,51 - 0,69	0,62	0,17
Th	3,4	-	11,0	1,7
Ti	52,5	39,9 - 65,1	56,4	12,5
V	5,08	3,97 - 6,19	5,40	0,38
W	13,3	11,4 - 15,2	12,7	5,0
Zn	247	207 - 287	261	41
Zr	59	-	55	6,6

Table 6.4: Comparison of U_3O_8-Standard ES 2 with SSMS

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error at 95% CL
Al	115	93 - 137	120	24
B	3,8	3,3 - 4,3	3,5	0,7
Bi	5,3	4,2 - 6,3	5,6	1,5
Ca	108	97 - 119	163	32
Cd	2,7	2,4 - 3,0	3,0	0,7
Co	13,5	12,0 - 14,9	13,9	1,1
Cr	59	36 - 82	65	11
Cu	54,1	43,7 - 64,4	58,3	5,7
Dy	0,56	0,43 - 0,69	0,69	0,16
Eu	0,39	0,30 - 0,48	0,49	0,14
Fe	208	165 - 251	264	53
Gd	0,47	0,29 - 0,65	0,64	0,42
In	5,3	3,8 - 6,8	6,4	1,1
K	180	162 - 199	171	35
Li	9,51	7,70 - 11,3	10,8	3,1
Mg	21,8	18,7 - 24,8	22,9	6,2
Mn	25,1	21,6 - 28,7	29,0	4,5
Mo	2,0	1,7 - 2,4	2,4	0,6
Ni	97,4	87,3 - 107	92,0	11,1
Sb	8,0	6,6 - 9,4	10,0	1,9
Si	75	59 - 90	77	17
Sm	0,59	0,50 - 0,68	0,66	0,32
Th	0,6	-	5,5	0,58
Ti	25,2	19,1 - 31,2	26,7	4,4
V	2,03	1,55 - 2,51	2,18	0,25
W	5,7	5,0 - 6,4	5,3	2,37
Zn	98,4	82,2 - 115	95,9	14,1
Zr	49		46	5

Table 6.5: *Comparison of U_3O_8-Standard ES 3 with SSMS*

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error at 95% CL
Al	68	54 - 81	68	18
B	1,4	1,2 - 1,6	1,3	0,3
Bi	3,8	3,0 - 4,6	4,9	1,7
Ca	72	65 - 79	99	20
Cd	1,0	0,9 - 1,2	1,3	0,3
Co	5,1	4,5 - 5,7	5,8	0,6
Cr	28	17 - 40	29	7
Cu	34,0	27,4 - 40,5	38,3	5,6
Dy	0,48	0,36 - 0,60	0,54	0,21
Eu	0,39	0,30 - 0,48	0,50	0,11
Fe	72	56 - 89	65	16
Gd	0,22	0,12 - 0,32	0,74	0,20
In	4,3	3,0 - 5,5	5,7	1,0
K	87	78 - 96	79	22
Li	7,12	5,75 - 8,49	7,86	2,1
Mg	11,4	9,8 - 13,0	15,9	4,9
Mn	12,1	10,4 - 13,8	13,3	2,1
Mo	1,2	1,0 - 1,4	1,3	0,3
Ni	53,9	48,3 - 59,6	52,2	8,2
Sb	3,9	3,1 - 4,7	5,2	1,2
Si	44	33 - 54	63	21
Sm	0,43	0,36 - 0,50	0,56	0,20
Th	0,3	-	3,0	0,5
Ti	10,9	8,3 - 13,6	10,1	2,0
V	1,01	0,74 - 1,28	1,22	0,12
W	4,2	3,6 - 4,7	3,7	1,6
Zn	54,8	45,6 - 63,9	62,7	7,6
Zr	49	-	46	6

Table 6.6: Comparison of U_3O_8-Standard ES 4 with SSMS

Element	Certified conc value (μg X /gU)	Confidence interval 95 % CL	SSMS conc value (μg X /gU)	Std Error at 95% CL
Al	23	19 - 28	27	5
B	0,6	0,5 - 0,7	0,8	0,1
Bi	2,5	1,9 - 3,0	3,1	0,8
Ca	23,8	21,2 - 26,4	34,1	5,7
Cd	0,5	-	1,5	0,4
Co	2,7	2,4 - 3,0	3,5	0,3
Cr	16	9 - 23	19	3
Cu	11,4	9,1 - 13,6	14,2	1,8
Dy	0,40	0,30 - 0,50	0,59	0,16
Eu	0,37	0,28 - 0,46	0,51	0,13
Fe	29	21 - 37	40	8
Gd	0,24	0,13 - 0,35	0,90	0,38
In	2,5	1,7 - 3,3	4,7	0,7
K	48	43 - 53	46	12
Li	3,25	2,60 - 3,90	3,73	0,44
Mg	5,4	4,6 - 6,2	8,8	2,2
Mn	5,73	4,9 - 6,6	7,24	1,32
Mo	5,3	4,5 - 6,2	6,7	0,9
Ni	23,2	20,7 - 25,7	25,0	2,5
Sb	1,6	1,2 - 2,0	4,2	0,7
Si	13	8 - 19	31	8
Sm	0,41	0,35 - 0,47	0,59	0,10
Th	-	-	1,1	0,2
Ti	5,5	4,2 - 6,9	6,3	1,1
V	0,44	0,29 - 0,59	0,79	0,17
W	2,8	2,4 - 3,2	3,3	1,5
Zn	22,9	18,9 - 26,8	29,0	4,0
Zr	40		37	3,4

Table 6.7: Comparison of U_3O_8-Standard ES 5 with SSMS

Element	Certified conc value (µg X /gU)	Confidence interval 95 % CL	SSMS conc value (µg X /gU)	Std Error of 95% CL
Al	12	0 - 15	14	3,4
B	0,4	0,30 - 0,40	0,9	0,2
Bi	0,6	0,5 - 0,8	1,6	0,6
Ca	11	9,7 - 12,3	29	6,7
Cd	0,1	-	0,64	0,2
Co	2,6	2,3 - 2,9	3,8	0,5
Cr	12	7 - 17	12	2
Cu	6,2	5,0 - 7,5	8,5	0,8
Dy	0,23	0,16 - 0,30	0,50	0,38
Eu	0,22	0,16 - 0,28	0,36	0,08
Fe	19	13 - 25	24	5
Gd	0,16	0,08 - 0,20	0,39	0,02
In	1,8	1,2 - 2,4	3,1	0,5
K	20	17 - 22	22	7
Li	1,86	1,47 - 2,25	2,37	0,86
Mg	2,4	2,0 - 2,8	5,9	1,7
Mn	3,09	2,6 - 3,6	4,8	0,9
Mo	20,9	17,6 - 24,2	24,4	2,6
Ni	12,8	11,4 - 14,2	15,4	2,0
Sb	0,5	0,3 - 0,8	2,6	0,6
Si	-	-	85	33
Sm	0,18	0,14 - 0,22	0,30	0,26
Th	-	-	0,71	0,2
Ti	3,1	2,3 - 3,9	4,5	0,8
V	0,14	0,05 - 0,23	0,39	0,1
W	0,9	0,8 - 1,1	1,2	1,0
Zn	13,2	10,8 - 15,6	18,1	3,3
Zr	27	-	23	2

CHAPTER SEVEN

GENERAL COMMENTS AND CONCLUSIONS

The success of the project for the development of analytical and data interpretation methods for the qualitative and quantitative analysis of trace impurities in uranium compounds with spark-source mass spectrometry has been adequately demonstrated.

Not only did the mass spectrometry results contribute to the characterisation of the internal U_3O_8 *impurity standards, but the analytical data was in many cases closer to the expected values than those of any of the other analytical techniques.*

Furthermore, the ability to analyse UF_4 *materials provided analytical results which could not be obtained with any other technique available at the time.*

The use of the ratio between singly and doubly charged exposure values as well as the use of the mean exposure value for the internal standard to determine whether a photoplate is acceptable or not, is a new approach to data interpretation in spark-source mass spectrometry. In this way possible misleading results can be directly avoided. Other quality assurance data interpretation methods have also been introduced. This thesis is now being used as a reference document for the mass spectrometry laboratory.

Contamination is an ever present threat to elemental trace level analysis. An effective but expensive solution would be a laboratory conforming to class 100 requirements. A relatively inexpensive alternative has been implemented in this laboratory. A laminar flow cabinet, where a curtain of HEPA filtered air is induced at the opening, is used for all sample preparation steps. Due to the positive pressure of air within the cabinet no contamination in the form of dust can enter.

The apparent disadvantages of the spark-source mass spectrometric technique are:

1 *Successful use requires wide experience, both in the operation of equipment and in the reading and interpretation of spectra.*

2 *The instrument is essentially a comparator; for quantitative analyses, standards of composition similar to the material under analysis are required. Unknown samples therefore present a problem when quantitative results are required.*

3 *The accuracy and precision are not as high as for some spectroscopic methods, notably inductively coupled plasma mass spectrometry (ICP-MS). It should be realised that these techniques have their own unique limitations, for example, laser ablation has a big problem with point inhomogeneity.*

The use of spark-source mass spectrometry to analyse trace impurities in uranium compounds is still one of the most powerful techniques available. This is confirmed by the following advantages:

1 *The procedure is specific for the element being determined. Sources of interference can be unequivocally identified and in many cases eliminated.*

2 *Quantitative determination of traces of the elements in a powder sample can be achieved without any preliminary chemical treatment. All solid materials may be determined.*

3 *A permanent record is obtained on a photographic plate.*

4 *The technique may be applied to the determination of small quantities of added constituents or of traces of impurities to solid-state matrices where conventional methods of analysis are difficult, fail, or give less accurate results.*

5 *The information content of analytical data which can be utilised is vast. This compensates for the relatively high operation costs of the technique. A direct complete picture can be obtained for all major and minor elements with the analysis of a single sample. This is especially useful when characterising unknown samples as well as for semi-quantitative analyses. Quantitative analysis with alternative methods for the identified impurities can then be executed cost effectively.*

6 *All isotopes of an element are recorded on a photoplate with intensities according to their isotopic abundances which leads to undisputed confirmation that a particular element is present in the sample as an impurity.*

7 *The up-time and reliability of the instrument is a proven fact, making this technique comparable if not better than any other analytical technique in this field.*

Spark-source mass spectrometry today has wider applications than just for the analysis of uranium compounds. Fields in which this technique is actively used include biomedical [42], geological [43] and horticultural science [44], as well as agricultural and environmental sciences [45]. It continues to play a prominent role in the contemporary nuclear technology laboratory [46, 47].

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APPENDIX A

LINEAR REGRESSION FORMULAE [29]

$y = mx + c$

$$m = \frac{(n\sum_{j=1}^{n} x_j y_j) - [(\sum_{j=1}^{n} x_j)(\sum_{j=1}^{n} y_j)]}{(n\sum_{j=1}^{n} x_j^2) - (\sum_{j=1}^{n} x_j)^2}$$

$$s = \left(\frac{s_{yy} - m\, s_{xy}}{n-2}\right)^{½}$$

$$s_{yy} = (\sum_{j=1}^{n} y_j^2) - \frac{(\sum_{j=1}^{n} y_j)^2}{n}$$

$$s_{xx} = (\sum_{j=1}^{n} x_j^2) - \frac{(\sum_{j=1}^{n} x_j)^2}{n}$$

$$s_{xy} = (\sum_{j=1}^{n} x_j y_j) - \frac{(\sum_{j=1}^{n} x_j)(\sum_{j=1}^{n} y_j)}{n}$$

$$c = \left(\frac{\sum_{j=1}^{n} y_j}{n}\right) - m\left(\frac{\sum_{j=1}^{n} x_j}{n}\right)$$

$$s_m = \frac{s}{(s_{xx})^{½}}$$

$$s_c = \frac{s(\sum_{j=1}^{n} x_j^2)^{½}}{(n\, s_{xx})^{½}}$$

APPENDIX B

TABLE OF ATOMIC AND MOLECULAR LINES FOR SPARK SOURCE MASS SPECTROMETRY OF COMPLEX SAMPLE-GRAPHITE MIXES

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ABSTRACT

A detailed table of atomic and molecular mass spectral lines has been prepared to aid in the interpretation of interferences and assignment of spectral lines in complex spectra arising from the spark source analysis of natural insulating powders blended with graphite to sustain the RF spark. The compilation consisting of 3000 listings is particularly useful for multielement trace analysis of geological and biological solids. Included are carbides, oxides, polymers, multiply-charged ions, and other molecular species of several or more major and minor elements as well as a large number of trace elements.

INTRODUCTION

Spark source mass spectrometry is a useful technique for multielemental trace analysis of geological and biological solids. Such insulating materials are usually powdered and mixed with graphite to produce strong and conducting electrodes. However, the sparking of complex graphite mixes yields complicated spectra containing the carbides, oxides, polymers, multiply-charged ions, and other molecular species of several or more major and minor elements as well as a large number of trace elements.

The primary purpose of the following table is to aid in the interpretation of interferences and assignment of spectral lines in complex spectra arising from the spark source analysis of natural insulating powders in a graphite matrix. In a secondary sense, the table may also be applied to other sample types or even to other fields of mass spectrometry such as ion probe analysis where molecular species become relatively more important.

There are indeed other excellent mass tables available for general use, but they are limited for application to the specific problem as stated. More explicitly, the table of Owens and Sherman (1) is arranged by individual element with comprehensive coverage for certain kinds of species excluding carbides, oxides, and many molecular species. The table of Guthrie and Heath (2), albeit arranged by mass, excludes carbides, most oxides, charge-exchange species, and other species of interest. The aim herein is to include those species omitted in preceding tables but of possible interest in complex graphite systems, to arrange the table in order of ascending mass values, to include the relative abundance of each species listed, to indicate the theoretical resolution required to separate a listed species from a line of analytical value, and finally to be concise in format but comprehensive in scope. The latter requirement, has resulted in approximately 3000 listings each containing four data words and producing a text of approximately 12,000 words on a physical format of only thirteen pages.

The entire table was manually calculated, compiled, and typed and is therefore not meant as a manual of supercritical mass and abundance data, but merely as an interpretive and useful guide. The user must assume any liability of any kind incurred in the employment of this table. Further, no claim is made as to the existence or nonexistence of any species listed herein, nor to that of any species accidentally or purposely omitted.

EXPLANATION OF TABLE

Each listing consists of a row of four words starting with the name of the species and followed by the mass, abundance, and resolutional requirement of the named species respectively.

I. NOMENCLATURE OF SPECIES

The usual chemical notation is used to identify the elemental constuents of the species. A leading superscript refers to the nominal mass of the species and a trailing superscript refers to the positive charge of the species. The plus signs of the charge superscripts are omitted since all species are ions of positive charge. The charge superscript is omitted entirely for species having a single positive charge. A special two-digit charge superscript indicates a charge-exchange species where the first digit is the initial charge of the species before a charge-reducing collision and the second digit gives the resulting or final charge after collision. The general nomenclature and the special meaning of the nominal mass superscript are best illustrated by example.

I.A. Elementally Homogeneous Species

(a) ^{12}C : a singly-charged ion of carbon 12

(b) $^{12}C^{3}$: a triply-charged ion of carbon 12

(c) $^{12}C_2$: a homo-isotopic dimer of carbon and the only combination of carbon isotopes having a nominal mass of 24. (Absence of superscript = +1).

(d) $^{25}C_2^{2}$: a hetero-isotopic dimer of carbon having a +2 positive charge and containing all combinations of carbon isotopes having a nominal mass of 25. (Only one combination in this case).

(e) $^{86}Si_3$: a trimer of silicon containing all combinations of silicon isotopes giving a nominal mass of 86, ie, $^{86}Si_3 = (^{28}Si_2 + {}^{30}Si) + (^{28}Si + {}^{29}Si_2)$, where the parentheses indicate the combinations having the same nominal mass.

(f) $^{12}C^{32}$: a charge-exchange species of carbon 12 where the initial charge is +3 and the final charge is +2.

I.B. Elementally Heterogeneous Species

(a) ^{28}SiC : a monocarbide of silicon 28 and the only significant* combination of carbon and silicon isotopes having a nominal mass of 40.

(b) ^{41}SiC : all the combinations** of silicon and carbon isotopes having a nominal mass of 41, ie, $(^{29}Si + {}^{12}C)$ and $(^{28}Si + {}^{13}C)$.

(c) $^{28}Si_3C_2$: the only significant* combination of silicon and carbon isotopes having a nominal mass of 108, ie, there is only one silicon trimer of nominal mass 84 and only one carbon dimer of nominal mass 24.

(d) $^{109}Si_3C_2$: all the combinations** of silicon trimer and carbon dimer having a nominal mass of 109, ie, $(^{85}Si_3 + {}^{12}C_2)$ and $(^{28}Si_3 + {}^{25}C_2)$.

* The word 'significant' means that if a single combination of isotopes is cited, then it is either the only possible combination or a combination which accounts for 99.0% or more of the abundance of all possible combinations.

** The phrase 'all the combinations' means that the combinations included are either the only possible ones or that they cumulatively account for 99.0% or more of the abundance of all combinations.

The starred definitions have meaning in relation to the mass and abundance data following a cited species (see parts II and III).

II. MASS (second word)

The masses of singly-charged species are taken from the table of Guthrie and Heath (2) and are rounded to five decimal places. Some elements are known to less than five places while others are only approximated as indicated by a (/) following the last digit in the mass value. Polymeric and heterogeneous species have masses equal to the sum of the individual contributing masses. Charge-exchange masses are obtained by multiplying the singly-charged mass by a factor (m/n^2) where (m) is the initial and (n) the final charge of the ion. Multiply-charged ions have masses equal to the singly-charged mass divided by the integral number of positive charges.

For species containing more than one combination of isotopes (eg., I.A.e, I.B.b, and I.B.d), the mass is that of the combination of isotopes which is the most abundant, as opposed to masses of single combinations which are unequivocal. The grouping of combinations of isotopes of the same elements to produce a species of the same chemical formula was performed to reduce the number of listings and is based on the fact that the combinations in a group are not resolvable with present commercial apparatus which have resolutions of 10,000 maximum and 5,000 or less practical.

III. ABUNDANCE (third word)

Isotopic abundances are based on Guthrie and Heath (2). Abundances apply only to species of the same kind (same chemical formula, same charge, but possibly different exact masses). For example, ^{28}SiC at mass 39.97693 comprises 91.19% of the total amount of silicon carbide formed from all combinations of silicon and carbon isotopes, ^{41}SiC at mass 40.97649 accounts for 5.67%, etc. The abundance of ^{28}SiC is that of a single combination while that of ^{41}SiC is the sum of the abundances of more than one combination.

The abundances of molecular species which are elementally homogeneous are calculated using the binomial expansion according to Hill (3) or the equivalent probability formula given by Owens and Sherman (1) for polyatomic clusters:

$$RA = (A^aB^bC^c\ldots N^n)(M!)/(a!b!c!..n!) \qquad 1.$$

where RA is the relative abundance of a given polyatomic cluster (a specified combination of isotopes) containing M total atoms of an element which has isotopes A', B', C',....N' with isotopic abundances A, B, C, ...N respectively and where the number of atoms of each isotope contained in the cluster is a, b, c, ...n respectively. The summation (a+b+c+...n) is equal to M. This formula is applied to each specific combination of isotopes until all possible combinations are exhausted.

For clusters containing different elements, the above formula is applied to each element individually and the abundance of the heterogeneous cluster is taken as the product of the indivual RA's for each element in the cluster.

The tabled abundances are given in percent. The appearance of an (E) in the tabled abundance indicates a negative exponential form so that 1.2E3, for example, means 00.0012%.

For species containing more than one combination (seeI), the abundance is the sum of all combinations considered, whereas the mass is that of the most abundant combination.

IV. RESOLUTIONAL REQUIREMENT (fourth word)

Resolution is defined as $R = M_o/\Delta M$. M_o is indicated in the table by a series of five dashes for a line of interest at each nominal mass unit and at some half-mass units where appropriate. A negative value for R indicates that the listed species occurs at a lower mass than M_o, the latter being indicated by the next dashed line. A positive value of R indicates a higher mass than M_o which is defined as the first previous dashed line.

The appearance of an (E) in the resolution value indicates a positive exponential form so that 15E3, for example, means a resolution of 15,000. There are no exponential forms for resolutions less than 10,000 (= 10E3).

V. SCOPE

The number and kinds of species included for each element depends on its definition as a major, minor, or trace constituent in geological and biological samples. Carbon, being the matrix considered, is defined as a major element. Other defined majors are oxygen, sodium, silicon, phosphorous, sulfur, potassium, calcium, titanium, and iron. Minors are given as chromium, nickel, zinc, strontium, zirconium, and barium. Most other elements are defined as trace.

For trace elements the species considered are: singly-and-multiply charged ions up to +3, polymerization up to the dimer only, mono-and-dicarbides, and mono-and-di-oxides.

For minor elements the species are: singly-and-multiply charged ions up to +4, polymerization up to the trimer, formation of oxide up to the trioxide and carbide to the tricarbide, and charge-exchange species with initial charges of +4 or less.

Major elements have more extensive coverage: singly-and-multiply charged ion up to +6, polymerization up to four atoms, formation of tetra-oxide and tetra-carbide, charge-exchange species with initial charge of 7 or less, and some complex species having two atoms of the major species and one to three atoms of carbon or oxygen. Polymer formers such as carbon, aluminum, and silicon are considered to form even more complex species and some combinations of these elements with other major elements are included. Appropriate higher degrees of polymerization and carbide and oxide formation are listed for these three elements.

Only the lower-charged species of rare gases are considered.

Hydrocarbons up to mass 100 are included.

The first hydrides(MH) of all elements from lithium to molybdenum plus barium, lanthanum, and cerium are also listed.

The mass range covered is from 1 to 270 with reductions in the number of entries from mass 210 to 270 where only two elements, thorium and uranium, are of interest.

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$^{1}\mathrm{H}$	1.00782	99.985	
$^{3}\mathrm{He}^{2}$	1.50801	01.4E4	
$^{12}\mathrm{C}^{6}$	2.00000	98.893	- 143
$^{4}\mathrm{He}^{2}$	2.00130	99.999	- 157
$^{6}\mathrm{Li}^{3}$	2.00500	07.42	- 221
$^{2}\mathrm{D}$	2.01410	00.015	-----
$^{1}\mathrm{H}_{2}$	2.01565	99.970	+1300
$^{13}\mathrm{C}^{6}$	2.16723	01.107	
$^{12}\mathrm{C}^{76}$	2.33328	99.893	
$^{7}\mathrm{Li}^{3}$	2.33870	92.58	
$^{13}\mathrm{C}^{76}$	2.52837	01.107	
$^{13}\mathrm{C}^{5}$	2.60067	01.107	
$^{16}\mathrm{O}^{6}$	2.66582	99.759	
$^{14}\mathrm{N}^{5}$	2.80061	99.634	
$^{17}\mathrm{O}^{6}$	2.83319	00.037	
$^{12}\mathrm{C}^{65}$	2.88000	98.893	
$^{18}\mathrm{O}^{6}$	2.99986	00.204	- 186
$^{12}\mathrm{C}^{4}$	3.00000	98.893	- 187
$^{9}\mathrm{Be}^{3}$	3.00407	100.000	- 252
$^{6}\mathrm{Li}^{2}$	3.00756	07.42	- 356
$^{3}\mathrm{He}$	3.01603	01.4E4	-----
$^{3}\mathrm{H}$	3.01605	......	+15E4
$^{3}\mathrm{H}_{2}$	3.02193	00.030	+ 512
$^{16}\mathrm{O}^{76}$	3.11051	99.759	
$^{13}\mathrm{C}^{65}$	3.12080	01.107	
$^{16}\mathrm{O}^{5}$	3.19898	99.759	
$^{13}\mathrm{C}^{4}$	3.25084	01.107	
$^{17}\mathrm{O}^{76}$	3.30531	00.037	
$^{10}\mathrm{Be}^{3}$	3.33765	19.61	
$^{17}\mathrm{O}^{5}$	3.39982	00.037	
$^{18}\mathrm{O}^{76}$	3.49976	00.204	- 437
$^{14}\mathrm{N}^{4}$	3.50077	99.634	- 485
$^{7}\mathrm{Li}^{2}$	3.50800	92.58	-----
$^{18}\mathrm{O}^{5}$	3.59983	00.204	
$^{11}\mathrm{B}^{3}$	3.66977	80.39	
$^{12}\mathrm{C}^{54}$	3.75000	98.893	
$^{15}\mathrm{N}^{4}$	3.75003	00.366	
$^{23}\mathrm{Na}^{6}$	3.83163	100.000	
$^{16}\mathrm{O}^{65}$	3.83878	99.759	
$^{24}\mathrm{Mg}^{6}$	3.99751	78.70	- 786
$^{16}\mathrm{O}^{4}$	3.99873	99.759	-1034
$^{12}\mathrm{C}^{3}$	4.00000	98.893	-1540
$^{4}\mathrm{He}$	4.00260	99.999	-----
$^{2}\mathrm{H}_{2}$	4.02820	02.0E4	+ 156
$^{13}\mathrm{C}^{54}$	4.06355	01.107	
$^{17}\mathrm{O}^{65}$	4.07979	00.037	
$^{25}\mathrm{Mg}^{6}$	4.16431	10.13	
$^{17}\mathrm{O}^{4}$	4.24978	00.037	
$^{18}\mathrm{O}^{65}$	4.31980	00.204	
$^{26}\mathrm{Mg}^{6}$	4.33043	11.17	- 829
$^{13}\mathrm{C}^{3}$	4.33445	01.107	-----
$^{14}\mathrm{N}^{54}$	4.37596	99.634	
$^{27}\mathrm{Al}^{6}$	4.49692	100.000	-1570
$^{18}\mathrm{O}^{4}$	4.49979	00.204	-----
$^{9}\mathrm{Be}^{2}$	4.50610	100.000	+ 713
$^{23}\mathrm{Na}^{5}$	4.59796	100.000	
$^{28}\mathrm{Si}^{6}$	4.66282	92.21	- 960
$^{14}\mathrm{N}^{3}$	4.66769	99.634	-----
$^{19}\mathrm{F}^{4}$	4.74960	100.000	
$^{24}\mathrm{Mg}^{5}$	4.79717	78.70	
$^{29}\mathrm{Si}^{6}$	4.82941	04.70	
$^{30}\mathrm{Si}^{6}$	4.99563	03.09	-----
$^{25}\mathrm{Mg}^{5}$	4.99717	10.13	+3240
$^{16}\mathrm{O}^{54}$	4.99841	99.759	+1797
$^{15}\mathrm{N}^{3}$	5.00004	00.366	+1130
$^{10}\mathrm{B}^{2}$	5.00647	19.61	+ 461
$^{31}\mathrm{P}^{6}$	5.16229	100.000	
$^{26}\mathrm{Mg}^{5}$	5.19652	11.17	
$^{17}\mathrm{O}^{54}$	5.31223	00.037	- 275
$^{32}\mathrm{S}^{6}$	5.32868	95.0	-1801
$^{16}\mathrm{O}^{3}$	5.33164	99.759	-----
$^{12}\mathrm{C}^{43}$	5.33333	98.893	+3149
$^{33}\mathrm{S}^{6}$	5.49524	00.76	- 585
$^{11}\mathrm{B}^{2}$	5.50465	80.39	-----
$^{28}\mathrm{Si}^{5}$	5.59539	92.21	
$^{18}\mathrm{O}^{54}$	5.62474	00.204	
$^{34}\mathrm{S}^{6}$	5.66131	04.22	-1120
$^{17}\mathrm{O}^{3}$	5.66638	00.037	-----
$^{23}\mathrm{Na}^{4}$	5.74745	100.000	-----
$^{24}\mathrm{Mg}^{65}$	5.75641	78.70	+ 642
$^{13}\mathrm{C}^{43}$	5.77926	01.107	+ 181
$^{28}\mathrm{Si}^{5}$	5.79530	04.70	

$^{36}\mathrm{S}^{6}$	5.99451	00.014	- 292
$^{36}\mathrm{A}^{6}$	5.99459	00.337	- 293
$^{30}\mathrm{Si}^{5}$	5.99475	03.09	- 295
$^{24}\mathrm{Mg}^{4}$	5.99626	78.70	- 319
$^{25}\mathrm{Mg}^{65}$	5.99660	10.13	- 327
$^{18}\mathrm{O}^{3}$	5.99972	00.204	- 391
$^{12}\mathrm{C}^{2}$	6.00000	98.893	- 398
$^{6}\mathrm{Li}$	6.01512	07.42	-----
$^{31}\mathrm{P}^{5}$	6.19476	100.000	
$^{14}\mathrm{N}^{43}$	6.22358	99.634	- 273
$^{26}\mathrm{Mg}^{65}$	6.23582	11.17	- 587
$^{25}\mathrm{Mg}^{4}$	6.24646	10.13	-----
$^{19}\mathrm{F}^{3}$	6.33280	100.000	
$^{32}\mathrm{S}^{5}$	6.39441	95.0	
$^{27}\mathrm{Al}^{65}$	6.47557	100.000	- 323
$^{39}\mathrm{K}^{6}$	6.49395	93.10	-3820
$^{26}\mathrm{Mg}^{4}$	6.49565	11.17	-----
$^{13}\mathrm{C}^{2}$	6.50168	01.107	+1077
$^{33}\mathrm{S}^{5}$	6.59429	00.76	
$^{40}\mathrm{A}^{6}$	6.66040	99.6	-22E4
$^{40}\mathrm{Ca}^{6}$	6.66043	96.97	-----
$^{40}\mathrm{K}^{6}$	6.66067	00.012	+27E3
$^{20}\mathrm{Ne}^{3}$	6.66415	90.92	+1790
$^{12}\mathrm{C}^{53}$	6.66666	98.893	+1064
$^{28}\mathrm{Si}^{65}$	6.71446	92.21	
$^{27}\mathrm{Al}^{4}$	6.74538	100.000	
$^{34}\mathrm{S}^{5}$	6.79358	100.000	
$^{41}\mathrm{K}^{6}$	6.82697	06.88	
$^{29}\mathrm{Si}^{65}$	6.95436	04.70	
$^{42}\mathrm{Ca}^{6}$	6.99310	00.64	- 306
$^{35}\mathrm{Cl}^{5}$	6.99377	75.529	- 316
$^{28}\mathrm{Si}^{4}$	6.99423	92.21	- 322
$^{21}\mathrm{Ne}^{3}$	6.99795	00.257	- 389
$^{14}\mathrm{N}^{2}$	7.00154	99.638	- 485
$^{7}\mathrm{Li}$	7.01600	92.58	-----
$^{6}\mathrm{LiH}$	7.02282	07.42	+1029
$^{16}\mathrm{O}^{43}$	7.10885	99.759	
$^{43}\mathrm{Ca}^{6}$	7.15980	00.146	
$^{23}\mathrm{Na}^{54}$	7.18431	100.000	-----
$^{30}\mathrm{Si}^{65}$	7.19370	03.09	+ 765
$^{36}\mathrm{S}^{5}$	7.19342	00.014	+ 789
$^{36}\mathrm{A}^{5}$	7.19351	00.337	+ 781
$^{13}\mathrm{C}^{53}$	7.22409	01.107	
$^{29}\mathrm{Si}^{4}$	7.24412	04.70	
$^{44}\mathrm{Ca}^{6}$	7.32592	02.06	-----
$^{22}\mathrm{Ne}^{3}$	7.33046	08.82	+1614
$^{37}\mathrm{Cl}^{5}$	7.39318	24.471	
$^{31}\mathrm{P}^{65}$	7.43370	100.000	
$^{45}\mathrm{Sc}^{6}$	7.49265	100.000	-9490
$^{30}\mathrm{Si}^{4}$	7.49344	03.09	-----
$^{24}\mathrm{Mg}^{54}$	7.49533	78.70	+3965
$^{15}\mathrm{N}^{2}$	7.50005	00.366	+1134
$^{17}\mathrm{O}^{43}$	7.55170	00.037	
$^{32}\mathrm{S}^{65}$	7.67330	95.0	
$^{31}\mathrm{P}^{4}$	7.74344	100.000	
$^{39}\mathrm{K}^{5}$	7.79274	93.10	-----
$^{25}\mathrm{Mg}^{54}$	7.80807	10.13	+ 508
$^{47}\mathrm{Ti}^{6}$	7.82529	07.29	+ 240
$^{48}\mathrm{Ti}^{6}$	7.99132	73.98	-1303
$^{48}\mathrm{Ca}^{6}$	7.99209	00.185	-1489
$^{40}\mathrm{A}^{5}$	7.99248	99.6	-1606
$^{40}\mathrm{Ca}^{5}$	7.99252	96.97	-1619
$^{40}\mathrm{K}^{5}$	7.99280	00.012	-1717
$^{32}\mathrm{S}^{4}$	7.99302	95.0	-1801
$^{24}\mathrm{Mg}^{3}$	7.99501	78.70	-3264
$^{16}\mathrm{O}^{2}$	7.99746	99.759	-----
$^{18}\mathrm{O}^{43}$	7.99963	00.204	+3685
$^{7}\mathrm{LiH}$	8.02382	92.57	+ 303
$^{26}\mathrm{Mg}^{54}$	8.11956	11.17	
$^{34}\mathrm{S}^{65}$	8.15229	04.22	-1434
$^{49}\mathrm{Ti}^{6}$	8.15798	05.51	-----
$^{41}\mathrm{K}^{5}$	8.19237	06.88	
$^{33}\mathrm{S}^{4}$	8.24287	00.76	
$^{50}\mathrm{Ti}^{6}$	8.24287	05.34	-1847
$^{50}\mathrm{Cr}^{6}$	8.32434	04.31	-1950
$^{50}\mathrm{V}^{6}$	8.32453	00.24	-2040
$^{25}\mathrm{Mg}^{3}$	8.32861	10.13	-----
$^{42}\mathrm{Ca}^{5}$	8.39173	00.64	+ 132
$^{27}\mathrm{Al}^{54}$	8.43173	100.00	-----
$^{19}\mathrm{F}^{43}$	8.44373	100.00	+ 703
$^{51}\mathrm{V}^{6}$	8.49066	99.76	- 954
$^{34}\mathrm{S}^{4}$	8.49197	04.22	-1118
$^{17}\mathrm{O}^{2}$	8.49957	00.037	-----

$^{43}\mathrm{Ca}^{5}$	8.59176	00.146	
$^{52}\mathrm{Cr}^{6}$	8.65675	83.76	-2107
$^{26}\mathrm{Mg}^{3}$	8.66086	11.17	-----
$^{35}\mathrm{Cl}^{4}$	8.74221	75.529	-----
$^{28}\mathrm{Si}^{54}$	8.75279	92.21	+ 826
$^{44}\mathrm{Ca}^{5}$	8.79110	02.06	
$^{53}\mathrm{Cr}^{6}$	8.82344	09.55	
$^{16}\mathrm{O}^{53}$	8.88606	99.759	
$^{54}\mathrm{Cr}^{6}$	8.98981	02.38	- 403
$^{54}\mathrm{Fe}^{6}$	8.98993	05.82	- 405
$^{45}\mathrm{Sc}^{5}$	8.99118	100.000	- 429
$^{36}\mathrm{S}^{4}$	8.99177	00.014	- 441
$^{36}\mathrm{A}^{4}$	8.99189	00.337	- 444
$^{27}\mathrm{Al}^{3}$	8.99384	100.000	- 491
$^{18}\mathrm{O}^{2}$	8.99958	00.204	- 714
$^{12}\mathrm{C}^{32}$	9.00000	98.893	- 739
$^{9}\mathrm{Be}$	9.01219	100.000	-----
$^{29}\mathrm{Si}^{54}$	9.05515	04.70	+ 210
$^{55}\mathrm{Mn}^{6}$	9.15634	100.000	
$^{46}\mathrm{Ti}^{5}$	9.19053	08.00	-----
$^{46}\mathrm{Ca}^{5}$	9.19074	00.003	+44E3
$^{37}\mathrm{Cl}^{4}$	9.24148	24.471	
$^{56}\mathrm{Fe}^{6}$	9.32249	91.66	-2961
$^{28}\mathrm{Si}^{3}$	9.32564	92.21	-----
$^{39}\mathrm{K}^{65}$	9.35129	93.10	- 604
$^{30}\mathrm{Si}^{54}$	9.36680	03.09	-----
$^{47}\mathrm{Ti}^{5}$	9.39075	07.29	
$^{17}\mathrm{O}^{53}$	9.44396	00.037	
$^{57}\mathrm{Fe}^{6}$	9.48923	02.19	- 953
$^{38}\mathrm{A}^{4}$	9.49068	00.063	-1115
$^{19}\mathrm{F}^{2}$	9.49920	100.000	-----
$^{48}\mathrm{Ti}^{5}$	9.58959	73.98	-----
$^{48}\mathrm{Ca}^{5}$	9.59051	00.185	+10E3
$^{44}\mathrm{Ca}^{65}$	9.59102	02.06	+6706
$^{58}\mathrm{Fe}^{6}$	9.65555	00.33	-2945
$^{58}\mathrm{Ni}^{6}$	9.65589	69.18	-3285
$^{29}\mathrm{Si}^{3}$	9.65883	04.70	-----
$^{31}\mathrm{P}^{54}$	9.67930	100.00	+ 472
$^{39}\mathrm{K}^{4}$	9.74093	93.10	-----
$^{13}\mathrm{C}^{32}$	9.75252	01.107	+ 840
$^{49}\mathrm{Ti}^{5}$	9.78957	05.51	
$^{59}\mathrm{Co}^{6}$	9.82221	100.000	-----
$^{41}\mathrm{K}^{65}$	9.83084	93.10	+1138
$^{60}\mathrm{Ni}^{6}$	9.98846	26.23	- 409
$^{50}\mathrm{Ti}^{5}$	9.98896	05.34	- 418
$^{50}\mathrm{Cr}^{5}$	9.98921	04.31	- 422
$^{50}\mathrm{V}^{5}$	9.98943	00.24	- 426
$^{32}\mathrm{S}^{54}$	9.99127	95.0	- 462
$^{20}\mathrm{Ne}^{2}$	9.99622	90.92	- 599
$^{18}\mathrm{O}^{53}$	9.99953	00.204	- 747
$^{10}\mathrm{B}$	10.01294	19.61	-----
$^{10}\mathrm{Be}$	10.01354	-----	+17E3
$^{9}\mathrm{BeH}$	10.02001	99.985	+1416
$^{61}\mathrm{Ni}^{6}$	10.15518	01.19	
$^{51}\mathrm{V}^{5}$	10.18880	99.76	
$^{23}\mathrm{Na}^{43}$	10.21767	100.000	
$^{41}\mathrm{K}^{4}$	10.24046	06.88	
$^{62}\mathrm{Ni}^{6}$	10.32139	03.66	-3226
$^{31}\mathrm{P}^{3}$	10.32459	100.00	-----
$^{52}\mathrm{Cr}^{6}$	10.38810	83.76	
$^{63}\mathrm{Cu}^{6}$	10.48827	60.09	-7547
$^{42}\mathrm{Ca}^{4}$	10.48966	00.64	-----
$^{21}\mathrm{Ne}^{2}$	10.49692	00.257	+1445
$^{14}\mathrm{N}^{32}$	10.50231	99.634	+ 829
$^{44}\mathrm{Ca}^{65}$	10.54932	02.06	
$^{53}\mathrm{Cr}^{5}$	10.58813	09.55	
$^{34}\mathrm{S}^{54}$	10.61496	04.22	
$^{64}\mathrm{Ni}^{6}$	10.65466	01.08	-3947
$^{64}\mathrm{Zn}^{6}$	10.65486	48.89	-4263
$^{32}\mathrm{S}^{3}$	10.65736	95.0	-----
$^{24}\mathrm{Mg}^{43}$	10.66002	78.70	+1702
$^{43}\mathrm{Ca}^{4}$	10.73970	00.146	- 224
$^{54}\mathrm{Cr}^{5}$	10.78777	02.38	-72E3
$^{54}\mathrm{Fe}^{5}$	10.78792	05.82	-----
$^{65}\mathrm{Cu}^{6}$	10.82130	30.91	+ 323
$^{55}\mathrm{Mn}^{5}$	10.98761	100.00	- 507
$^{66}\mathrm{Zn}^{6}$	10.98768	27.81	- 509
$^{44}\mathrm{Ca}^{4}$	10.98887	02.06	- 539
$^{33}\mathrm{S}^{3}$	10.99049	00.76	- 585
$^{22}\mathrm{Ne}^{2}$	10.99569	08.82	- 808
$^{11}\mathrm{B}$	11.00931	80.39	-----
$^{10}\mathrm{BH}$	11.02076	19.61	+ 962
$^{46}\mathrm{Ti}^{65}$	11.02863	08.00	+ 570

$^{25}\mathrm{Mg}^{43}$	11.10482	10.13	
$^{67}\mathrm{Zn}^{6}$	11.15452	04.11	- 344
$^{56}\mathrm{Fe}^{5}$	11.18699	91.66	-----
$^{45}\mathrm{Sc}^{4}$	11.23898	100.00	
$^{47}\mathrm{Ti}^{65}$	11.26842	07.29	
$^{68}\mathrm{Zn}^{6}$	11.32081	18.57	-6256
$^{34}\mathrm{S}^{3}$	11.32262	04.22	-----
$^{57}\mathrm{Fe}^{5}$	11.38703	02.19	
$^{69}\mathrm{Ga}^{6}$	11.48762	60.4	-1581
$^{46}\mathrm{Ti}^{4}$	11.48816	08.00	-1708
$^{46}\mathrm{Ca}^{4}$	11.48842	00.003	-1777
$^{23}\mathrm{Na}^{2}$	11.49489	100.000	-----
$^{48}\mathrm{Ti}^{65}$	11.50751	73.98	+ 911
$^{26}\mathrm{Mg}^{43}$	11.54782	11.17	
$^{58}\mathrm{Fe}^{5}$	11.58666	00.33	-28E3
$^{58}\mathrm{Ni}^{5}$	11.58707	69.18	-----
$^{70}\mathrm{Ge}^{6}$	11.65400	20.52	-5112
$^{70}\mathrm{Zn}^{6}$	11.65422	00.62	-5658
$^{35}\mathrm{Cl}^{3}$	11.65628	75.529	-----
$^{47}\mathrm{Ti}^{4}$	11.73794	07.29	
$^{59}\mathrm{Co}^{5}$	11.78664	100.00	
$^{71}\mathrm{Ga}^{6}$	11.82080	39.6	
$^{60}\mathrm{Ni}^{5}$	11.98615	26.23	- 866
$^{50}\mathrm{Ti}^{65}$	11.98675	05.45	- 906
$^{72}\mathrm{Ge}^{6}$	11.98693	27.43	- 918
$^{48}\mathrm{Ti}^{4}$	11.98699	73.98	- 922
$^{50}\mathrm{Cr}^{65}$	11.98705	04.31	- 927
$^{48}\mathrm{Ca}^{4}$	11.98813	00.185	-1011
$^{36}\mathrm{S}^{3}$	11.98903	00.014	-1094
$^{36}\mathrm{A}^{3}$	11.98913	00.337	-1110
$^{27}\mathrm{Al}^{43}$	11.99180	100.00	-1463
$^{24}\mathrm{Mg}^{2}$	11.99252	78.70	-1604
$^{16}\mathrm{O}^{32}$	11.99619	99.759	-3150
$^{12}\mathrm{C}$	12.00000	98.893	-----
$^{11}\mathrm{BH}$	12.01713	80.38	+ 701
$^{6}\mathrm{Li}_2$	12.03000	00.551	+ 400
$^{73}\mathrm{Ge}^{6}$	12.15389	07.76	- 547
$^{39}\mathrm{K}^{54}$	12.17616	93.10	-----
$^{61}\mathrm{Ni}^{5}$	12.18622	01.19	+1210
$^{49}\mathrm{Ti}^{4}$	12.23697	05.51	
$^{74}\mathrm{Ge}^{6}$	12.32017	36.54	-6845
$^{74}\mathrm{Se}^{6}$	12.32042	00.87	-7950
$^{37}\mathrm{Cl}^{3}$	12.32197	24.471	-----
$^{62}\mathrm{Ni}^{5}$	12.38567	03.66	
$^{28}\mathrm{Si}^{43}$	12.43418	92.21	
$^{52}\mathrm{Cr}^{65}$	12.46752	83.76	- 459
$^{50}\mathrm{Ti}^{4}$	12.48620	05.45	-1859
$^{50}\mathrm{Cr}^{4}$	12.48651	04.31	-1949
$^{50}\mathrm{V}^{4}$	12.48679	00.24	-2038
$^{75}\mathrm{As}^{6}$	12.48695	100.00	-2093
$^{40}\mathrm{Ca}^{54}$	12.48831	96.97	-2710
$^{25}\mathrm{Mg}^{2}$	12.49292	10.13	-----
$^{63}\mathrm{Cu}^{5}$	12.58592	69.09	
$^{38}\mathrm{A}^{3}$	12.65424	00.063	
$^{53}\mathrm{Cr}^{65}$	12.70576	09.55	- 448
$^{51}\mathrm{V}^{4}$	12.73599	99.76	-----
$^{17}\mathrm{O}^{32}$	12.74935	00.037	+ 953
$^{23}\mathrm{Na}^{53}$	12.77209	100.00	- 931
$^{64}\mathrm{Ni}^{5}$	12.78559	01.08	-53E3
$^{64}\mathrm{Zn}^{5}$	12.78583	48.89	-----
$^{41}\mathrm{K}^{54}$	12.80057	06.88	+ 867
$^{29}\mathrm{Si}^{43}$	12.87843	04.70	
$^{54}\mathrm{Cr}^{65}$	12.94533	02.38	- 224
$^{54}\mathrm{Fe}^{65}$	12.94551	05.82	- 225
$^{52}\mathrm{Cr}^{4}$	12.98513	83.76	- 713
$^{65}\mathrm{Cu}^{5}$	12.98556	30.91	- 731
$^{39}\mathrm{K}^{3}$	12.98790	93.10	- 841
$^{26}\mathrm{Mg}^{2}$	12.99130	11.17	-1078
$^{13}\mathrm{C}$	13.00336	01.107	-----
$^{12}\mathrm{CH}$	13.00782	98.878	+2916
$^{13}\mathrm{Li}_2$	13.03112	13.74	+ 468
$^{55}\mathrm{Mn}^{65}$	13.18513	100.00	- 265
$^{66}\mathrm{Zn}^{5}$	13.18521	27.81	- 265
$^{53}\mathrm{Cr}^{4}$	13.23516	09.55	-----
$^{40}\mathrm{A}^{3}$	13.32080	99.60	-22E4
$^{40}\mathrm{Ca}^{3}$	13.32086	96.97	-----
$^{40}\mathrm{K}^{3}$	13.32133	00.012	+28E3
$^{30}\mathrm{Si}^{43}$	13.32166	03.09	+17E3
$^{24}\mathrm{Mg}^{53}$	13.32502	78.70	+3202
$^{67}\mathrm{Zn}^{5}$	13.38543	04.11	
$^{56}\mathrm{Fe}^{65}$	13.42439	91.66	
$^{54}\mathrm{Cr}^{4}$	13.48472	02.38	-2230
$^{54}\mathrm{Fe}^{4}$	13.48490	05.82	-2298
$^{27}\mathrm{Al}^{2}$	13.49077	100.00	-----
$^{18}\mathrm{O}^{32}$	13.49937	00.204	+1569

$^{68}\mathrm{Zn}^{5}$	13.58497	18.57	
$^{41}\mathrm{K}^{3}$	13.65394	06.88	-----
$^{57}\mathrm{Fe}^{65}$	13.66450	02.19	+1293
$^{55}\mathrm{Mn}^{4}$	13.73451	100.00	-----
$^{44}\mathrm{Ca}^{54}$	13.73609	02.06	+8693
$^{31}\mathrm{P}^{43}$	13.76612	100.00	+ 434
$^{69}\mathrm{Ga}^{5}$	13.78514	60.4	+ 271
$^{58}\mathrm{Fe}^{65}$	13.90400	00.33	
$^{56}\mathrm{Fe}^{4}$	13.98374	91.66	- 724
$^{70}\mathrm{Ge}^{5}$	13.98480	20.52	- 766
$^{70}\mathrm{Zn}^{5}$	13.98508	00.62	- 778
$^{43}\mathrm{Ca}^{3}$	13.98621	00.64	- 831
$^{28}\mathrm{Si}^{2}$	13.98847	92.21	- 959
$^{14}\mathrm{N}$	14.00307	99.634	-----
$^{14}\mathrm{C}$	14.00324	LT.01	+82E3
$^{13}\mathrm{CH}$	14.01118	01.107	+1726
$^{12}\mathrm{CH}_2$	14.01565	98.863	+1113
$^{7}\mathrm{Li}_2$	14.03200	85.71	+ 484
$^{32}\mathrm{S}^{43}$	14.20981	95.0	- 593
$^{57}\mathrm{Fe}^{4}$	14.23385	02.19	-----
$^{19}\mathrm{F}^{32}$	14.24880	100.00	+ 952
$^{46}\mathrm{Ti}^{54}$	14.36020	08.00	
$^{43}\mathrm{Ca}^{3}$	14.31959	00.146	
$^{26}\mathrm{Mg}^{53}$	14.43477	11.17	
$^{58}\mathrm{Fe}^{4}$	14.48333	00.33	-2945
$^{58}\mathrm{Ni}^{4}$	14.48384	69.18	-3256
$^{29}\mathrm{Si}^{2}$	14.48825	04.70	-----
$^{44}\mathrm{Ca}^{3}$	14.65183	02.06	-----
$^{47}\mathrm{Ti}^{54}$	14.67242	07.29	+ 713
$^{59}\mathrm{Co}^{4}$	14.73330	100.00	
$^{60}\mathrm{Ni}^{4}$	14.98269	26.23	- 861
$^{48}\mathrm{Ti}^{54}$	14.98373	73.98	- 916
$^{45}\mathrm{Sc}^{3}$	14.98531	100.00	-1014
$^{30}\mathrm{Si}^{2}$	14.98688	03.09	-1134
$^{27}\mathrm{Al}^{53}$	14.98974	100.00	-1446
$^{15}\mathrm{N}$	15.00011	00.366	-----
$^{12}\mathrm{CH}_3$	15.02347	98.523	+ 642
$^{14}\mathrm{NH}$	15.01090	99.509	+1390
$^{34}\mathrm{S}^{43}$	15.09683	04.22	
$^{61}\mathrm{Ni}^{4}$	15.23277	01.19	
$^{46}\mathrm{Ti}^{3}$	15.31754	08.00	-43E3
$^{46}\mathrm{Ca}^{3}$	15.31790	00.003	-----
$^{62}\mathrm{Ni}^{4}$	15.48209	03.66	-3233
$^{31}\mathrm{P}^{2}$	15.48688	100.00	-----
$^{35}\mathrm{Cl}^{43}$	15.54171	75.529	-15E3
$^{28}\mathrm{Si}^{53}$	15.54274	92.21	-----
$^{50}\mathrm{Ti}^{54}$	15.60775	05.34	-----
$^{50}\mathrm{Cr}^{54}$	15.60814	04.31	+40E3
$^{63}\mathrm{Cu}^{4}$	15.73240	69.09	
$^{47}\mathrm{Ti}^{3}$	15.65059	07.29	
$^{64}\mathrm{Ni}^{4}$	15.98199	01.08	-1238
$^{64}\mathrm{Zn}^{4}$	15.98229	48.89	-1267
$^{48}\mathrm{Ti}^{3}$	15.98265	73.98	-1305
$^{48}\mathrm{Ca}^{3}$	15.98413	00.185	-1481
$^{32}\mathrm{S}^{2}$	15.98604	95.0	-1803
$^{16}\mathrm{O}$	15.99491	99.759	-----
$^{15}\mathrm{NH}$	16.00793	00.366	+1229
$^{14}\mathrm{NH}_2$	16.01872	99.955	+ 671
$^{12}\mathrm{CH}_4$	16.03130	98.344	+ 400
$^{29}\mathrm{Si}^{53}$	16.09805	04.70	
$^{52}\mathrm{Cr}^{54}$	16.23141	83.76	-30E3
$^{65}\mathrm{Cu}^{4}$	16.23195	30.91	-----
$^{49}\mathrm{Ti}^{3}$	16.31596	05.51	
$^{66}\mathrm{Zn}^{4}$	16.48151	27.81	-3907
$^{33}\mathrm{S}^{2}$	16.48573	00.76	-----
$^{53}\mathrm{Cr}^{54}$	16.54395	09.55	
$^{50}\mathrm{Ti}^{3}$	16.64826	05.34	-----
$^{50}\mathrm{Cr}^{3}$	16.64868	04.31	+40E3
$^{50}\mathrm{V}^{3}$	16.64905	00.24	+21E3
$^{30}\mathrm{Si}^{53}$	16.65209	03.09	+4347
$^{67}\mathrm{Zn}^{4}$	16.73178	04.11	
$^{54}\mathrm{Cr}^{54}$	16.85590	02.38	-----
$^{54}\mathrm{Fe}^{54}$	16.85613	05.82	+73E3
$^{68}\mathrm{Zn}^{4}$	16.98122	18.57	- 949
$^{51}\mathrm{V}^{3}$	16.98133	99.76	- 955
$^{34}\mathrm{S}^{2}$	16.98393	04.22	-1118
$^{17}\mathrm{O}$	16.99913	00.037	-----
$^{16}\mathrm{OH}$	17.00274	99.747	+4709
$^{14}\mathrm{NH}_3$	17.02655	99.593	+ 620
$^{55}\mathrm{Mn}^{54}$	17.16814	100.000	
$^{31}\mathrm{P}^{53}$	17.20765	100.000	
$^{23}\mathrm{Na}^{32}$	17.24234	100.000	
$^{52}\mathrm{Cr}^{3}$	17.31350	83.76	-----
$^{39}\mathrm{K}^{43}$	17.31720	93.10	+4679

$^{56}\mathrm{Fe}^{54}$	17.47967	91.66	-3680
$^{70}\mathrm{Zn}^{4}$	17.48134	00.62	-5677
$^{35}\mathrm{Cl}^{2}$	17.48442	75.529	-----
$^{53}\mathrm{Cr}^{3}$	17.64688	09.55	
$^{40}\mathrm{Ca}^{43}$	17.76115	96.97	-----
$^{32}\mathrm{S}^{53}$	17.76226	95.0	+16E3
$^{57}\mathrm{Fe}^{54}$	17.79231	02.19	+ 570
$^{54}\mathrm{Cr}^{3}$	17.97962	02.38	- 921
$^{54}\mathrm{Fe}^{3}$	17.97987	05.82	- 933
$^{36}\mathrm{S}^{2}$	17.98354	00.014	-1152
$^{36}\mathrm{A}^{2}$	17.98377	00.337	-1170
$^{24}\mathrm{Mg}^{32}$	17.98878	78.70	-1734
$^{18}\mathrm{O}$	17.99916	00.204	-----
$^{12}\mathrm{C}_3^2$	18.00000	96.71	+21E3
$\mathrm{H}_2\mathrm{O}$	18.01056	99.747	+1579
$^{6}\mathrm{LiC}$	18.01500	07.34	+1136
$^{9}\mathrm{Be}_2$	18.02439	100.00	+ 713
$^{14}\mathrm{NH}_4$	18.03437	99.584	+ 511
$^{58}\mathrm{Fe}^{54}$	18.10416	00.33	
$^{41}\mathrm{K}^{43}$	18.20526	06.88	
$^{55}\mathrm{Mn}^{3}$	18.31269	100.00	
$^{37}\mathrm{Cl}^{2}$	18.48295	24.471	-----
$^{37}\mathrm{C}_3^2$	18.50168	3.25	+ 987
$^{56}\mathrm{Fe}^{3}$	18.64498	91.66	
$^{25}\mathrm{Mg}^{32}$	18.73938	10.13	
$^{34}\mathrm{S}^{53}$	18.87103	04.22	
$^{57}\mathrm{Fe}^{3}$	18.97847	02.19	- 953
$^{38}\mathrm{A}^{2}$	18.98137	00.063	-1116
$^{19}\mathrm{F}$	18.99840	100.00	-----
$^{38}\mathrm{C}_3^2$	19.00336	00.036	+3830
$^{18}\mathrm{OH}$	19.00698	00.204	+2214
$\mathrm{H}_2\mathrm{O}$	19.01477	00.037	+1161
$^{19}\mathrm{LiC}$	19.01600	91.64	+1079
$\mathrm{H}_3\mathrm{O}$	19.01837	99.714	+ 951
$^{58}\mathrm{Fe}^{3}$	19.31110	00.33	-28E3
$^{58}\mathrm{Ni}^{3}$	19.31178	69.18	-----
$^{39}\mathrm{K}^{2}$	19.48186	93.10	-----
$^{26}\mathrm{Mg}^{32}$	19.48695	11.17	+3827
$^{44}\mathrm{Ca}^{43}$	19.53577	02.06	+ 361
$^{60}\mathrm{Ni}^{3}$	19.97692	26.23	-1288
$^{40}\mathrm{A}^{2}$	19.98119	99.60	-1777
$^{40}\mathrm{Ca}^{2}$	19.98129	96.97	-1793
$^{40}\mathrm{K}^{2}$	19.98200	00.012	-1915
$^{20}\mathrm{Ne}$	19.99244	90.92	-----
HF	20.00622	99.985	+1451
$\mathrm{H}_2\mathrm{O}$	20.01480	00.204	+ 894
$^{10}\mathrm{B}_2$	20.02588	03.85	+ 598
$^{27}\mathrm{Al}^{32}$	20.23616	100.00	
$^{61}\mathrm{Ni}^{3}$	20.31036	01.19	
$^{46}\mathrm{Ti}^{43}$	20.42339	08.00	
$^{41}\mathrm{K}^{2}$	20.48092	06.88	
$^{62}\mathrm{Ni}^{3}$	20.64278	03.66	
$^{47}\mathrm{Ti}^{43}$	20.86745	07.29	
$^{63}\mathrm{Cu}^{3}$	20.97653	69.09	-1212
$^{84}\mathrm{Sr}^{4}$	20.97831	00.56	-1351
$^{42}\mathrm{Ca}^{2}$	20.97931	00.64	-1444
$^{28}\mathrm{Si}^{32}$	20.98270	92.21	-1883
$^{21}\mathrm{Ne}$	20.99385	00.257	-----
$^{9}\mathrm{BeC}$	21.01219	98.89	+1144
$^{21}\mathrm{B}_2$	21.02225	31.52	+ 739
$^{85}\mathrm{Rb}^{4}$	21.22801	72.15	
$^{64}\mathrm{Ni}^{3}$	21.30932	01.08	-55E3
$^{64}\mathrm{Zn}^{3}$	21.30971	48.89	-----
$^{48}\mathrm{Ti}^{43}$	21.31020	73.98	+43E3
$^{86}\mathrm{Sr}^{4}$	21.47734	09.86	-11E3
$^{43}\mathrm{Ca}^{2}$	21.47939	00.146	-----
$^{65}\mathrm{Cu}^{3}$	21.64259	30.91	-----
$^{39}\mathrm{K}^{53}$	21.64650	93.10	+5535
$^{87}\mathrm{Sr}^{4}$	21.72725	09.36	-27E4
$^{87}\mathrm{Rb}^{4}$	21.72733	27.85	-----
$^{29}\mathrm{Si}^{32}$	21.73237	04.70	+4311
$^{66}\mathrm{Zn}^{3}$	21.97535	27.81	-9157
$^{88}\mathrm{Sr}^{4}$	21.97650	82.56	-18E3
$^{44}\mathrm{Ca}^{2}$	21.97775	02.06	-----
$^{22}\mathrm{Ne}$	21.99138	08.82	+1612
$^{6}\mathrm{LiO}$	22.00991	07.40	+ 683
$^{10}\mathrm{BC}$	22.01294	19.39	+ 625
$^{11}\mathrm{B}_2$	22.01861	64.63	+ 538
$^{50}\mathrm{Ti}^{43}$	22.19768	05.34	- 773
$^{50}\mathrm{Cr}^{43}$	22.19824	04.31	- 788
$^{40}\mathrm{Ca}^{53}$	22.20143	96.97	- 339
$^{89}\mathrm{Y}^{4}$	22.22643	100.00	-----
$^{67}\mathrm{Zn}^{3}$	22.30905	04.11	

$^{90}Zr^{4}$	22.47608	51.48	-12E3
$^{45}Sc^{2}$	22.47796	100.00	-----
$^{30}Si^{32}$	22.48032	03.09	+9524
$^{68}Zn^{3}$	22.64162	18.57	
$^{91}Zr^{4}$	22.72633	11.22	-----
$^{41}K^{53}$	22.75657	06.88	+ 753
$^{69}Ga^{3}$	22.97524	60.4	-1581
$^{92}Zr^{4}$	22.97617	17.11	-1689
$^{46}Ti^{2}$	22.97632	08.00	-1708
$^{46}Ca^{2}$	22.97684	00.003	-1776
^{23}Na	22.98978	100.00	-----
^{23}BC	23.00931	79.72	+1177
^{7}LiO	23.01091	92.36	+1089
$^{52}Cr^{43}$	23.08467	83.76	
$^{93}Nb^{4}$	23.22642	100.00	-----
$^{31}P^{32}$	23.23032	100.00	+5955
$^{70}Ge^{3}$	23.30800	20.52	-----
$^{70}Zn^{3}$	23.30845	00.62	+52E3
$^{47}Ti^{2}$	23.47587	07.29	-----
$^{94}Zr^{4}$	23.47691	17.40	+23E3
$^{53}Cr^{43}$	23.52918	09.55	
$^{71}Ga^{3}$	23.64033	39.6	
$^{54}Cr^{43}$	23.97283	02.38	-1964
$^{54}Fe^{43}$	23.97316	05.82	-2019
$^{72}Ge^{3}$	23.97386	27.43	-2145
$^{48}Ti^{2}$	23.97397	73.98	-2167
$^{48}Ca^{2}$	23.97626	00.185	-2731
$^{96}Zr^{4}$	23.97733	02.80	-3111
$^{32}S^{32}$	23.97906	95.0	-4011
^{24}Mg	23.98504	78.70	-----
^{23}NaH	23.99760	99.985	+1910
$^{12}C_2$	24.00000	97.798	+1603
$^{73}Ge^{3}$	24.30778	07.76	
$^{55}Mn^{43}$	24.41691	100.00	-8690
$^{44}Ca^{53}$	24.41972	02.06	-----
$^{49}Ti^{2}$	24.47393	05.51	
$^{74}Ge^{3}$	24.64033	36.54	-----
$^{74}Se^{3}$	24.64085	00.87	+47E3
$^{56}Fe^{43}$	24.85997	91.66	
$^{50}Ti^{2}$	24.97239	05.34	-1858
$^{50}Cr^{2}$	24.97302	04.31	-1949
$^{50}V^{2}$	24.97358	00.24	-2038
$^{75}As^{3}$	24.97390	100.00	-2093
^{25}Mg	24.98584	10.13	-----
^{24}MgH	24.99760	78.69	+3559
$^{25}C_2$	25.00336	02.189	+1426
^{9}BeO	25.00711	99.759	+1175
$^{12}C_2H$	25.00782	97.786	+1137
$^{57}Fe^{43}$	25.30462	02.19	-10E3
$^{76}Se^{3}$	25.30643	09.02	-38E3
$^{76}Ge^{3}$	25.30710	07.76	-----
$^{51}V^{2}$	25.47199	99.76	-----
$^{34}S^{32}$	25.47590	04.22	+6515
$^{51}C_4^{2}$	25.50502	5.4E4	+ 771
$^{46}Ti^{53}$	25.52924	08.00	+ 445
$^{77}Se^{3}$	25.64000	07.58	
$^{58}Fe^{43}$	25.74814	00.33	
$^{52}Cr^{2}$	25.97026	83.76	-2107
$^{78}Se^{3}$	25.97246	23.52	-2565
$^{78}Kr^{3}$	25.97340	00.354	-2827
^{26}Mg	25.98259	11.17	-----
^{25}MgH	25.99366	10.13	+2347
^{12}CN	26.00307	98.54	+1269
$^{13}C_2$	26.00671	00.013	+1077
^{10}BO	26.00785	19.56	+1029
$^{12}C_2H_2$	26.01565	97.77	+ 786
$^{47}Ti^{53}$	26.08431	07.29	
$^{59}Co^{43}$	26.19252	100.00	- 769
$^{35}Cl^{32}$	26.22664	75.529	-----
$^{79}Br^{3}$	26.30613	50.537	
$^{53}Cr^{2}$	26.47032	09.55	
$^{60}Ni^{43}$	26.63590	26.23	-9123
$^{80}Se^{3}$	26.63882	49.82	-----
$^{80}Kr^{3}$	26.63886	02.27	+67E4
$^{48}Ti^{53}$	26.63775	73.98	-25E3
$^{54}Cr^{2}$	26.96944	02.38	-2230
$^{54}Fe^{2}$	26.96980	05.82	-2298
$^{81}Br^{3}$	26.97214	49.463	-2870
^{27}Al	26.98154	100.00	-----
^{26}MgH	26.99041	11.17	+3042
$^{12}C^{15}N$	27.00011	00.362	+1453
^{11}BO	27.00422	80.20	+1190
$^{13}C^{14}N$	27.00643	01.107	+1084
$^{12}C_2H_3$	27.02347	97.762	+ 643
$^{82}Kr^{3}$	27.30448	11.56	-26E3
$^{82}Se^{3}$	27.30554	09.19	-----
$^{55}Mn^{2}$	27.46903	100.00	
$^{83}Kr^{3}$	27.63802	11.55	
$^{50}Ti^{53}$	27.74710	05.34	-39E3
$^{50}Cr^{53}$	27.74781	04.31	-----
$^{56}Fe^{2}$	27.96747	91.66	-2957
$^{63}Cu^{43}$	27.96871	69.09	-3404
$^{84}Kr^{3}$	27.97050	56.90	-4351
$^{84}Sr^{3}$	27.97108	00.56	-4782
^{28}Si	27.97693	92.21	-----
^{27}AlH	27.98936	99.985	+2251
^{12}CO	27.99491	98.66	+1556
$^{14}N_2$	28.00615	99.269	+ 957
$^{12}C_2H_4$	28.03130	97.75	+ 524
$^{85}Rb^{3}$	28.30401	72.15	
$^{64}Zn^{43}$	28.41295	48.89	
$^{57}Fe^{2}$	28.46770	02.19	
$^{86}Sr^{3}$	28.63645	09.86	-----
$^{86}Kr^{3}$	28.63693	17.37	+60E3
$^{52}Cr^{53}$	28.85584	83.76	-----
$^{65}Cu^{43}$	28.85679	30.91	+30E3
$^{58}Fe^{2}$	28.96666	00.33	-2948
$^{58}Ni^{2}$	28.96768	69.18	-3289
$^{87}Sr^{3}$	28.96966	07.02	-4242
$^{87}Rb^{3}$	28.96977	27.85	-4312
^{29}Si	28.97649	04.70	-----
^{28}SiH	28.98475	92.20	+3508
^{13}CO	28.99827	01.104	+1330
$^{12}C^{17}O$	28.99910	00.037	+1282
^{12}CHO	29.00274	98.64	+1104
$^{29}N_2$	29.00318	00.73	+1086
$^{12}C_2H_5$	29.03912	97.74	+ 463
$^{39}K^{32}$	29.22278	93.10	
$^{88}Sr^{3}$	29.30200	82.56	
$^{53}Cr^{53}$	29.41147	09.55	
$^{59}Co^{2}$	29.46659	100.00	
$^{89}Y^{3}$	29.63524	100.00	
$^{60}Ni^{2}$	29.96538	26.23	-3577
$^{54}Cr^{53}$	29.96604	02.38	-3883
$^{54}Fe^{53}$	29.96645	05.82	-4100
$^{90}Zr^{3}$	29.96881	51.48	-5305
$^{40}Ca^{32}$	29.97194	96.97	-16E3
^{30}Si	29.97376	03.09	-----
^{29}SiH	29.98431	04.70	+2841
^{14}NO	29.99799	99.39	+1237
$^{12}C^{18}O$	29.99916	00.202	+1180
$^{60}C_5^{2}$	30.00000	94.57	+1142
$^{15}N_2$	30.00022	00.001	+1133
$^{12}CH_2O$	30.01056	99.63	+ 815
$^{6}LiC_2$	30.01500	07.26	+ 727
$^{12}C_2H_6$	30.04695	97.73	+ 410
$^{91}Zr^{3}$	30.30177	11.22	
$^{61}Ni^{2}$	30.46554	01.19	
$^{55}Mn^{53}$	30.52114	100.00	
$^{69}Ga^{43}$	30.63365	60.4	-25E3
$^{92}Zr^{3}$	30.63489	17.11	-----
$^{92}Mo^{3}$	30.63618	15.84	+24E3
$^{41}K^{32}$	30.72137	06.88	
$^{62}Ni^{2}$	30.96417	03.66	-3230
$^{93}Nb^{3}$	30.96855	100.00	-5945
^{31}P	30.97376	100.00	-----
^{30}SiH	30.98158	03.09	+3961
^{15}NO	30.99502	00.362	+1457
^{12}CF	30.99840	98.893	+1257
^{13}CO	31.00251	00.002	+1077
$^{62}C_5^{2}$	31.00336	00.119	+1046
$^{31}LiC_2$	31.01600	90.70	+ 733
$^{12}CH_3O$	31.01839	98.62	+ 694
$^{56}Fe^{53}$	31.07497	91.66	
$^{94}Mo^{3}$	31.30198	09.04	-55E3
$^{94}Zr^{3}$	31.30255	17.40	-----
$^{63}Cu^{2}$	31.46480	69.09	
$^{63}C_5^{2}$	31.50502	00.0013	
$^{57}Fe^{53}$	31.63078	02.19	-7849
$^{95}Mo^{3}$	31.63481	15.72	-----
$^{64}Ni^{2}$	31.96398	01.08	-3952
$^{64}Zn^{2}$	31.96457	48.89	-4263
$^{96}Mo^{3}$	31.96832	16.53	-8526
$^{96}Ru^{3}$	31.9696	05.51	-13E3
$^{96}Zr^{3}$	31.96977	02.80	-14E3
^{32}S	31.97207	95.0	-----
^{31}PH	31.98158	99.985	+3362
$^{16}O_2$	31.98983	99.52	+1800
$^{13}C^{19}F$	32.00176	01.11	+1077
$^{12}CH_4O$	32.02613	99.60	+ 591
$^{58}Fe^{53}$	32.18517	00.33	
$^{97}Mo^{3}$	32.30207	09.46	
$^{65}Cu^{2}$	32.46389	30.91	-----
$^{130}Ba^{4}$	32.47656	00.101	+2562
$^{98}Mo^{3}$	32.63533	23.78	-----
$^{98}Ru^{3}$	32.651/	01.87	+2083
$^{74}Ge^{43}$	32.85378	36.54	
$^{66}Zn^{2}$	32.96302	27.81	-3907
$^{44}Ca^{32}$	32.96662	02.06	-6812
$^{99}Ru^{3}$	32.96868	12.72	-12E3
^{33}S	32.97146	00.76	-----
$^{132}Ba^{4}$	32.97628	00.097	+6841
^{32}SH	32.97989	95.0	+3911
$^{33}O_2$	32.99405	00.075	+1460
$^{100}Ru^{3}$	33.302/	12.62	-20E4
$^{100}Mo^{3}$	33.30217	09.63	-----
$^{67}Zn^{2}$	33.46357	04.11	-----
$^{134}Ba^{4}$	33.47606	02.42	+2679
$^{101}Ru^{3}$	33.635/	17.07	
$^{135}Ba^{4}$	33.72639	06.59	
$^{68}Zn^{2}$	33.96243	18.57	-6256
^{34}S	33.96786	04.22	-----
$^{102}Ru^{3}$	33.96791	31.61	+68E4
$^{102}Pd^{3}$	33.96829	00.96	+79E3
$^{136}Ba^{4}$	33.97609	07.81	+4127
^{33}SH	33.97928	00.76	+2974
$^{34}O_2$	33.99408	00.407	+1295
$^{10}BC_2$	34.01294	19.18	+ 754
$^{137}Ba^{4}$	34.22639	11.32	
$^{103}Rh^{3}$	34.30152	100.00	
$^{69}Ga^{2}$	34.46286	60.4	-----
$^{46}Ti^{32}$	34.46447	08.00	+21E3
$^{138}Ba^{4}$	34.47622	71.66	+2580
$^{104}Pd^{3}$	34.63443	10.97	-----
$^{104}Ru^{3}$	34.63474	18.58	+11E4
$^{139}La^{4}$	34.72651	99.911	
$^{70}Ge^{2}$	34.96200	20.52	-5105
$^{70}Zn^{2}$	34.96267	00.62	-5658
$^{105}Pd^{3}$	34.96827	22.23	-60E3
^{35}Cl	34.96885	75.529	-----
^{34}SH	34.97568	04.22	+5120
$^{140}Ce^{4}$	34.97632	88.48	+4681
^{23}NaC	34.98978	98.89	+1669
^{19}FO	34.99331	99.76	+1430
$^{35}O_2$	34.99829	1.4E4	+1188
$^{35}BC_2$	35.00931	79.05	+ 864
$^{47}Ti^{32}$	35.21382	07.29	
$^{106}Pd^{3}$	35.30097	27.33	-----
$^{106}Cd^{3}$	35.30198	01.215	+35E3
$^{71}Ga^{2}$	35.46241	39.6	-----
$^{142}Ce^{4}$	35.47733	11.07	+2377
$^{107}Ag^{3}$	35.63495	51.35	
$^{72}Ge^{2}$	35.96080	27.43	-5718
$^{48}Ti^{32}$	35.96096	73.98	-5867
^{36}S	35.96709	00.014	-----
^{36}A	35.96755	00.337	+79E3
$^{108}Pd^{3}$	35.96782	26.71	+49E3
$^{1}H^{35}Cl$	35.97668	75.52	+3750
^{24}MgC	35.98504	77.83	+2008
$^{23}Na^{13}C$	35.99314	01.107	+1378
$^{36}C_3$	36.00000	96.71	+1093
$(NH_4)_2$	36.06874	-----	+ 354
$^{109}Ag^{3}$	36.30154	48.65	
$^{73}Ge^{2}$	36.46167	07.76	
$^{110}Cd^{3}$	36.63443	12.39	-----
$^{110}Pd^{3}$	36.63482	11.81	+94E3
$^{74}Ge^{2}$	36.96050	36.54	-6846
$^{74}Se^{2}$	36.96127	00.87	-7984
^{37}Cl	36.96590	24.471	-----
$^{111}Cd^{3}$	36.96809	12.75	+17E3
^{36}SH	36.97491	00.014	+5120
^{37}MgC	36.98584	11.00	+1858
$^{37}C_3$	37.00336	03.25	+ 987
$^{12}C_3H$	37.00782	96.70	+ 882
$^{112}Cd^{3}$	37.30102	24.07	-----
$^{112}Sn^{3}$	37.3017	00.96	+55E3
$^{50}Ti^{32}$	37.45859	05.34	-17E3
$^{50}Cr^{32}$	37.45954	04.31	-28E3
$^{75}As^{2}$	37.46086	100.00	-----
$^{113}In^{3}$	37.63477	04.28	-----
$^{113}Cd^{3}$	37.63482	12.26	+75E4
$^{85}Rb^{43}$	37.73868	72.15	
$^{76}Se^{2}$	37.95964	09.02	-12E3
$^{76}Ge^{2}$	37.96065	07.76	-18E3
^{38}A	37.96273	00.063	-----
$^{114}Cd^{3}$	37.96785	28.86	+7415
$^{114}Sn^{3}$	37.9680	00.66	+7204
$^{1}H^{37}Cl$	37.97373	24.467	+3450
^{38}MgC	37.98269	11.16	+1910
$^{25}Mg^{13}C$	37.98920	00.112	+1434
$^{19}F_2$	37.99680	100.00	+1114
$^{38}C_3$	38.00670	00.036	+ 863
$^{12}C_2{}^{14}N$	38.00307	97.43	+ 941
$^{12}C_3H_2$	38.01565	96.69	+ 717

$^{115}Sn^{3}$	38.30112	00.35	-48E4
$^{115}In^{3}$	38.30120	95.72	-----
$^{77}Se^{2}$	38.45999	07.58	
$^{116}Sn^{3}$	38.63406	14.30	-----
$^{116}Cd^{3}$	38.63500	07.58	+41E3
$^{52}Cr^{32}$	38.95538	83.76	-4678
$^{78}Se^{2}$	38.95870	23.52	-7777
$^{78}Kr^{2}$	38.96010	00.354	-11E3
^{39}K	38.96371	93.10	-----
$^{117}Sn^{3}$	38.96770	07.61	+9765
^{27}AlC	38.98154	98.89	+2190
^{23}NaO	38.98469	99.76	+1856
$^{26}Mg^{13}C$	38.98605	00.124	+1748
$^{12}C_2{}^{15}N$	39.00011	00.362	+1070
$^{7}LiO_2$	39.00581	92.13	+ 926
$^{13}C_3$	39.01005	01.4E4	+ 841
$^{12}C_3H_3$	39.02347	96.70	+ 652
$^{88}Sr^{43}$	39.06934	82.56	
$^{118}Sn^{3}$	39.30068	24.03	
$^{79}Br^{2}$	39.45920	50.537	
$^{89}Y^{43}$	39.51365	100.00	
$^{119}Sn^{3}$	39.63438	08.58	
$^{53}Cr^{32}$	39.70549	09.55	
$^{90}Zr^{43}$	39.95748	51.46	-7820
$^{80}Se^{2}$	39.95824	49.82	-9187
$^{80}Kr^{2}$	39.95830	02.27	-9315
^{40}A	39.96239	99.60	-20E4
^{40}Ca	39.96259	96.97	-----
^{40}K	39.96400	00.012	+28E3
$^{120}Sn^{3}$	39.96740	32.85	+8308
$^{120}Te^{3}$	39.96816	00.089	+7175
^{39}KH	39.97153	93.09	+4470
^{28}SiC	39.97693	91.19	+2993
^{24}MgO	39.97996	78.60	+2301
$^{27}Al^{13}C$	39.98489	98.89	+1791
$^{12}C_2O$	39.99491	97.56	+1236
$^{12}C_3H_4$	40.03130	95.60	+ 582
$^{121}Sb^{3}$	40.30124	57.25	
$^{54}Cr^{32}$	40.45415	02.38	-9965
$^{54}Fe^{32}$	40.45471	05.82	-12E3
$^{81}Br^{2}$	40.45821	49.463	-----
$^{122}Te^{3}$	40.63430	02.46	-21E4
$^{122}Sn^{3}$	40.63449	04.72	-----
$^{92}Zr^{43}$	40.84652	17.11	
$^{82}Kr^{2}$	40.95673	11.56	-8032
$^{82}Se^{2}$	40.95832	09.19	-12E3
^{41}K	40.96183	06.88	-----
$^{123}Sb^{3}$	40.96806	42.75	+6575
$^{123}Te^{3}$	40.9681	00.87	+6533
^{40}CaH	40.97041	96.96	+4774
^{40}KH	40.97182	00.012	+4100
^{41}SiC	40.97649	05.67	+2792
$^{23}Na^{18}O$	40.98894	00.204	+1508
$^{12}C_2{}^{17}O$	40.99910	00.037	+1099
$^{12}C_2HO$	41.00274	97.55	+1001
$^{9}BeO_2$	41.0020	99.52	+1020
$^{12}C_3H_5$	41.0391	96.66	+ 530
$^{55}Mn^{32}$	41.20354	100.00	
$^{124}Te^{3}$	41.30104	04.61	-58E3
$^{124}Sn^{3}$	41.30175	05.94	-----
$^{124}Xe^{3}$	41.30204	00.096	+14E4
$^{83}Kr^{2}$	41.45703	11.55	
$^{125}Te^{3}$	41.63487	06.99	
$^{94}Zr^{43}$	41.73673	17.40	
$^{56}Fe^{32}$	41.95120	91.66	-5647
$^{84}Kr^{2}$	41.95576	56.90	-15E3
$^{84}Sr^{2}$	41.95663	00.56	-20E3
^{42}Ca	41.95863	00.64	-----
$^{126}Te^{3}$	41.96796	18.71	+4497
$^{126}Xe^{3}$	41.96815	00.90	+4407
^{41}KH	41.96965	06.88	+3807
^{42}SiC	41.97649	03.11	+2766
^{26}MgO	41.97751	11.11	+2222
$^{24}Mg^{18}O$	41.98420	00.16	+1641
$^{12}C_2{}^{18}O$	41.99916	97.56	+1035
$^{84}C^{2}_{7}$	42.00000	92.48	+1014
$^{10}BO_2$	42.00274	19.52	+ 951
$^{12}C_2H_2O$	42.01056	97.54	+ 808
$^{12}C_3H_6$	42.04695	96.64	+ 475
$^{127}I^{3}$	42.30155	100.00	
$^{85}Rb^{2}$	42.45601	72.15	-----
$^{85}C^{2}_{7}$	42.50168	07.25	+ 930
$^{128}Xe^{3}$	42.63450	01.919	-63E3
$^{128}Te^{3}$	42.63518	31.79	-----
$^{57}Fe^{32}$	42.70155	02.19	
$^{86}Sr^{2}$	42.95468	09.86	-10E3
$^{86}Kr^{2}$	42.95540	17.37	-13E3
^{43}Ca	42.95878	00.146	-----

^{43}Ca	42.95878	00.146	-----
^{42}CaH	42.96645	00.64	+5601
$^{129}Xe^{3}$	42.96825	26.44	+4536
^{31}PC	42.97376	98.89	+2860
^{27}AlO	42.97645	99.76	+2431
$^{30}Si^{13}C$	42.97711	00.034	+2332
$^{25}Mg^{18}O$	42.98530	00.021	+1620
$^{12}C_2{}^{19}F$	42.9984	97.80	+1450
$^{11}BO_2$	42.99911	80.00	+1065
C_2H_3O	43.01839	97.53	+ 721
$^{12}C_3H_7$	43.05477	96.63	+ 448
$^{130}Xe^{3}$	43.30117	04.08	-48E3
$^{130}Ba^{3}$	43.30208	00.101	-----
$^{130}Te^{3}$	43.30232	34.48	+18E4
$^{58}Fe^{32}$	43.44999	00.33	-9635
$^{87}Sr^{2}$	43.45450	07.02	-----
$^{87}Rb^{2}$	43.45465	27.85	+29E4
$^{131}Xe^{3}$	43.63503	21.18	
$^{88}Sr^{2}$	43.95301	82.56	-18E3
^{44}Ca	43.95550	02.06	-----
^{43}CaH	43.96660	00.146	+3960
$^{132}Ba^{3}$	43.96837	00.097	+3415
$^{132}Xe^{3}$	43.96805	26.89	+3502
^{28}SiO	43.97184	91.99	+2690
^{32}SC	43.97207	94.0	+2653
$^{31}P^{13}C$	43.97711	01.107	+2026
$^{26}Mg^{18}O$	43.98175	00.023	+1674
CO_2	43.98983	97.8	+1280
C_2H_4O	44.02621	97.51	+ 622
C_3H_8	44.06260	96.62	+ 410
$^{59}Co^{32}$	44.19989	100.00	
$^{133}Cs^{3}$	44.30171	100.00	
$^{89}Y^{2}$	44.45286	100.00	
$^{134}Ba^{3}$	44.63475	02.42	-----
$^{134}Xe^{3}$	44.63514	10.44	+11E4
$^{60}Ni^{32}$	44.94808	26.23	-5734
$^{90}Zr^{2}$	44.95217	51.46	-12E3
^{45}Sc	44.95592	100.00	-----
^{44}CaH	44.96332	02.06	+6075
$^{135}Ba_3$	44.96852	06.59	+3568
^{29}SiO	44.97141	04.69	+2902
^{45}SC	44.97542	01.80	+2305
^{27}AlO	44.98070	00.204	+1814
$^{45}CO_2$	44.99318	01.176	+1207
$^{12}C_2H_5O$	45.03404	97.50	+ 575
$^{136}Ba^{3}$	45.30146	07.81	-----
$^{136}Ce^{3}$	45.30236	00.193	+50E3
$^{136}Xe^{3}$	45.30240	08.87	+48E3
$^{91}Zr^{2}$	45.45266	11.22	
$^{137}Ba^{3}$	45.63519	11.32	
$^{92}Zr^{2}$	45.95234	17.11	-16E4
^{46}Ti	45.95263	08.00	-----
^{46}Ca	45.95369	03.3E3	+43E3
$^{92}Mo^{2}$	45.95428	15.84	+28E3
^{45}ScH	45.96374	99.985	+4136
^{34}SC	45.96786	04.17	+3017
$^{138}Ba^{3}$	45.96829	71.66	+2934
^{30}SiO	45.96867	03.08	+2865
$^{138}Ce^{3}$	45.96868	00.25	+2863
$^{138}La^{3}$	45.96891	00.089	+2823
$^{28}Si^{18}O$	45.97609	00.138	+1958
$^{23}Na_2$	45.97956	100.00	+1706
$^{14}NO_2$	45.99290	99.15	+1141
C_2H_6O	46.04136	97.49	+ 515
$^{139}La^{3}$	46.30201	99.911	
$^{93}Nb^{2}$	46.45283	100.000	
$^{140}Ce^{3}$	46.63509	88.48	
^{47}Ti	46.95176	07.29	-----
$^{94}Zr^{2}$	46.95382	17.40	+23E3
$^{94}Mo^{2}$	46.95297	09.04	+39E3
^{46}TiH	46.96045	08.00	+5403
^{31}PO	46.96872	99.76	+2768
^{35}ClC	46.96885	74.69	+2747
$^{141}Pr^{3}$	46.96916	100.00	+2698
$^{29}Si^{18}O$	46.97565	00.01	+1961
$^{23}NaC_2$	46.98978	97.80	+1234
$^{15}NO_2$	46.98991	00.36	+1231
$^{63}Cu^{32}$	47.19720	69.09	
$^{142}Nd^{3}$	47.30249	27.11	-78E3
$^{142}Ce^{3}$	47.30310	11.07	-----
$^{95}Mo^{2}$	47.45222	15.72	
$^{143}Nd^{3}$	47.63653	12.17	
$^{64}Zn^{32}$	47.94686	48.89	-44E3
^{48}Ti	47.94795	73.98	-----
$^{96}Mo^{2}$	47.95248	16.53	+11E3
^{48}Ca	47.95253	00.185	+10E3
$^{96}Ru^{2}$	47.9544	05.51	+7434
$^{96}Zr^{2}$	47.95465	02.80	+7156
^{47}TiH	47.95958	07.29	+4123
^{32}SO	47.96699	94.8	+2518

^{36}SC	47.96709	00.013	+2505
$^{144}Nd^{3}$	47.96993	23.85	+2181
$^{24}Mg_2$	47.97003	61.94	+2167
$^{144}Sm^{3}$	47.97055	03.09	+2122
$^{35}Cl^{13}C$	47.97220	00.34	+1977
$^{30}Si^{18}O$	47.97292	00.006	+1914
$^{16}O_3$	47.98473	99.28	+1304
$^{24}MgC_2$	47.98504	76.97	+1294
$^{12}C_4$	48.00000	95.63	+ 921
$^{145}Nd^{3}$	48.30402	08.30	
$^{97}Mo^{2}$	48.45311	09.46	
$^{97}C^{2}_{8}$	48.50168	07.25	
$^{146}Nd^{3}$	48.63756	17.22	-----
$^{65}Cu^{32}$	48.69534	30.91	+ 834
^{49}Ti	48.94787	05.51	-----
$^{98}Mo^{2}$	48.95299	23.78	+9560
^{48}TiH	48.95577	73.97	+6196
^{37}ClC	48.96590	24.20	+2715
^{49}SO	48.96640	00.80	+2641
$^{49}Mg_2$	48.97088	15.95	+2127
$^{147}Sm^{3}$	48.97150	14.97	+2071
$^{98}Ru^{2}$	48.977	01.87	+1680
$^{49}MgC_2$	48.98584	11.63	+1290
$^{49}O_3$	48.98892	00.11	+1192
$^{49}C_4$	49.00336	04.29	+ 882
$^{12}C_4H$	49.00782	95.62	+ 816
$^{148}Sm^{3}$	49.30481	11.24	-----
$^{148}Nd^{3}$	49.30549	05.73	+73E3
$^{99}Ru^{2}$	49.45303	12.72	
$^{149}Sm^{3}$	49.63893	13.83	
^{50}Ti	49.94479	05.34	-----
^{50}Cr	49.94605	04.31	+40E3
^{50}V	49.94716	00.24	+21E3
$^{100}Ru^{2}$	49.953	12.62	+6083
$^{100}Mo^{2}$	49.95326	09.63	+5897
^{49}TiH	49.95569	05.51	+4582
^{34}SO	49.96278	04.21	+2776
$^{50}Mg_2$	49.96763	18.61	+2187
^{37}ClC	49.96926	00.27	+2041
$^{23}NaAl$	49.97132	100.00	+1883
$^{150}Sm^{3}$	49.97230	07.44	+1815
$^{150}Nd^{3}$	49.97361	05.62	+1733
$^{50}MgC_2$	49.98259	11.16	+1321
$^{50}O_3$	49.98898	00.61	+1130
$^{12}CF_2$	49.99680	98.89	+ 960
$^{50}C_4$	50.00670	00.072	+ 806
$^{12}C_4H_2$	50.01564	95.61	+ 705
$^{151}Eu^{3}$	50.30651	47.82	
$^{101}Ru^{2}$	50.453	17.07	
$^{152}Sm^{3}$	50.63979	26.72	
$^{152}Gd^{3}$	50.63981	00.20	
^{51}V	50.94398	99.76	-----
$^{102}Ru^{2}$	50.95187	31.61	+6457
$^{102}Pd^{2}$	50.95243	00.96	+6029
^{50}TiH	50.95261	05.34	+5903
^{50}CrH	50.95387	04.31	+5151
^{39}KC	50.96371	92.07	+2582
^{35}ClO	50.96376	75.35	+2576
$^{24}MgAl$	50.96653	78.70	+2254
$^{28}SiNa$	50.96671	92.21	+2241
$^{51}Mg_2$	50.96843	02.26	+2084
$^{153}Eu^{3}$	50.9735	52.18	+1726
$^{27}AlC_2$	50.98154	97.80	+1358
$^{19}FO_2$	50.98822	99.52	+1152
$^{13}CF_2$	51.00016	01.11	+ 907
$^{51}C_4$	51.01005	05.4E4	+ 771
C_4H_3	51.02346	95.61	+ 641
$^{154}Gd^{3}$	51.30698	02.15	-16E4
$^{154}Sm^{3}$	51.30731	22.71	-----
$^{103}Rh^{2}$	51.45228	100.00	-----
$^{206}Pb^{4}$	51.49361	23.6	+1245
$^{155}Gd^{3}$	51.6409	14.73	-----
$^{69}Ga^{32}$	51.69428	60.4	+ 967
$^{207}Pb^{4}$	51.74397	22.6	
^{52}Cr	51.94051	83.76	-----
$^{104}Pd^{2}$	51.95164	10.97	+4667
^{51}VH	51.95180	99.985	+4601
$^{104}Ru^{2}$	51.95211	18.58	+4478
$^{28}SiMg$	51.96197	72.57	+2420
^{36}SO	51.96200	00.014	+2417
^{40}CaC	51.96259	95.90	+2352
$^{26}Mg_2$	51.96518	01.25	+2105
$^{25}MgAl$	51.96738	10.13	+1933
^{52}KC	51.96706	01.04	+1956
$^{156}Dy^{3}$	51.971/	00.052	+1704
$^{156}Gd^{3}$	51.97409	20.47	+1547
$^{28}SiC_2$	51.97693	90.18	+1427
$^{208}Pb^{4}$	51.99416	52.3	+ 968
$^{12}C_3O$	51.99492	96.48	+ 955
$^{12}C_4H_4$	52.03128	95.60	+ 572

$^{157}Gd^{3}$	52.3080	15.68	
$^{105}Pd^{2}$	52.45241	22.23	
$^{158}Dy^{3}$	52.64134	00.09	
$^{158}Gd^{3}$	52.6415	24.87	
^{53}Cr	52.94065	09.55	-----
^{52}CrH	52.94833	83.75	+6893
$^{106}Pd^{2}$	52.95146	27.33	+4897
$^{106}Cd^{2}$	52.95297	01.215	+4297
^{37}ClO	52.96081	24.41	+2626
^{41}KC	52.96183	06.80	+2500
$^{26}MgAl$	52.96413	11.17	+2255
$^{40}Ca^{13}C$	52.96594	01.07	+2093
$^{159}Tb^{3}$	52.97496	100.00	+1543
$^{53}SiC_2$	52.97649	06.61	+1477
C_4H_5	53.03910	95.05	+ 538
$^{160}Dy^{3}$	53.3080	02.294	-50E3
$^{160}Gd^{3}$	53.30907	21.90	-----
$^{107}Ag^{2}$	53.45242	51.35	
$^{161}Dy^{3}$	53.6419	18.88	
^{54}Cr	53.93887	02.38	-73E3
^{54}Fe	53.93961	05.82	-----
^{53}CrH	53.94847	09.55	+6088
$^{108}Pd^{2}$	53.95174	26.71	+4445
$^{108}Cd^{2}$	53.95204	00.875	+4338
^{42}CaC	53.95863	00.63	+2835
$^{27}Al_2$	53.96306	100.00	+2300
$^{41}K^{13}C$	53.96518	00.076	+2109
$^{54}SiC_2$	53.97376	03.12	+1577
$^{162}Dy^{3}$	53.9752	25.53	+1515
$^{162}Er^{3}$	53.97624	00.136	+1472
$^{12}C_9^{2}$	54.00000	90.44	+ 893
C_4H_6	54.04692	95.57	+ 499
$^{109}Ag^{2}$	54.45231	48.65	-----
$^{109}C_9^{2}$	54.50168	09.12	+1103
$^{164}Dy^{3}$	54.64283	28.18	-----
$^{164}Er^{3}$	54.64327	01.56	+12E4
$^{74}Ge^{32}$	54.69251	36.54	+1100
^{55}Mn	54.93805	100.00	-----
^{54}CrH	54.94699	02.38	+6359
^{54}FeH	54.94743	05.82	+5857
$^{110}Cd^{2}$	54.95165	12.39	+4040
$^{28}SiAl$	54.95847	92.88	+2990
$^{110}Pd^{2}$	54.95224	11.81	+3872
^{39}KO	54.95862	92.88	+2671
$^{165}Ho^{3}$	54.95862	100.00	+2671
^{55}CaC	54.95878	00.151	+2650
$^{31}PC_2$	54.97376	97.80	+1537
$^{23}NaO_2$	54.97960	99.52	+1322
$^{110}C_9^{2}$	55.00335	00.41	+ 841
$^{12}C_4H_7$	55.05474	95.56	+ 471
$^{166}Er^{3}$	55.3096	33.41	
$^{111}Cd^{2}$	55.45214	12.75	
$^{167}Er^{3}$	55.6435	22.94	
^{56}Fe	55.93494	91.66	-----
^{55}MnH	55.94587	99.985	+5118
$^{112}Cd^{2}$	55.95153	24.07	+3372
$^{112}Sn^{2}$	55.9526	00.96	+3167
$^{28}Si_2$	55.95386	85.03	+2956
^{44}CaC	55.95550	02.04	+2788
^{40}CaO	55.95750	96.51	+2479
$^{29}SiAl$	55.95803	04.70	+2422
^{40}KO	55.95891	00.018	+2334
$^{32}SC_2$	55.97207	92.91	+1506
$^{24}MgO_2$	55.97485	78.32	+1400
$^{168}Er^{3}$	55.9769	27.07	+1333
$^{168}Yb^{3}$	55.97797	00.135	+1300
C_4H_8	56.06256	95.55	+ 438
$^{169}Tm^{3}$	56.31145	100.00	
$^{113}In^{2}$	56.45215	04.28	-71E4
$^{113}Cd^{2}$	56.45223	12.26	-----
$^{170}Yb^{3}$	56.645/	03.03	-28E4
$^{170}Er^{3}$	56.6452	14.88	-----
^{57}Fe	56.93541	02.19	-----
^{56}FeH	56.94276	91.65	+7746
$^{114}Cd^{2}$	56.95178	28.86	+3478
$^{114}Sn^{2}$	56.9520	00.66	+3432
$^{57}Si_2$	56.95342	08.66	+3161
$^{30}SiAl$	56.95530	03.09	+2863
^{45}ScC	56.95592	98.89	+2776
^{41}KO	56.95674	06.86	+2669
$^{44}Ca^{13}C$	56.95835	00.023	+2482
$^{38}K^{18}O$	56.96287	00.19	+2071
$^{57}SC_2$	56.97542	02.82	+1423
$^{25}MgO_2$	56.97566	10.08	+1415
$^{171}Yb^{3}$	56.979/	14.31	+1306
C_4H_9	57.07038	95.54	+ 422
$^{172}Yb^{3}$	57.3084/	21.82	
$^{115}Sn^{2}$	57.45168	00.35	-44E4
$^{115}In^{2}$	57.45181	95.72	-----
$^{173}Yb^{3}$	57.646/	16.13	

^{58}Fe	57.93331	00.33	-28E3
^{58}Ni	57.93535	69.18	-----
^{57}FeH	57.94323	02.19	+7352
$^{58}Si_2$	57.95069	05.92	+3777
$^{116}Sn^{2}$	57.95110	14.30	+3678
$^{116}Cd^{2}$	57.95250	07.58	+3378
^{46}CaC	57.95369	03.3E3	+3159
^{46}TiC	57.95263	07.91	+3353
^{42}CaO	57.95340	00.64	+3208
$^{40}Ca^{18}O$	57.96202	00.20	+2172
$^{34}SC_2$	57.96786	04.13	+1782
$^{26}MgO_2$	57.97241	11.12	+1564
$^{174}Yb^{3}$	57.9752/	31.84	+1454
$^{23}Na_2C$	57.97976	98.89	+1305
$^{174}Hf^{3}$	57.980/	00.18	+1298
$^{175}Lu^{3}$	58.314/	97.41	
$^{117}Sn^{2}$	58.45155	07.61	
$^{176}Hf^{3}$	58.6469	05.20	-88E3
$^{176}Lu^{3}$	58.6473	02.59	-22E4
$^{176}Yb^{3}$	58.64757	12.73	-----
^{59}Co	58.93318	100.00	-----
^{58}FeH	58.94113	00.33	+7413
^{58}NiH	58.94317	69.17	+5899
$^{59}Si_2$	58.95025	00.30	+3452
^{28}SiP	58.95069	92.21	+3366
$^{118}Sn^{2}$	58.95103	24.03	+3302
^{59}TiC	58.95176	07.29	+3172
^{43}CaO	58.95369	00.146	+2873
$^{41}K^{18}O$	58.96099	00.014	+2118
$^{35}ClC_2$	58.96885	73.87	+1652
$^{27}AlO_2$	58.97136	99.52	+1544
$^{177}Hf^{3}$	58.9808	18.50	+1238
$^{23}NaC_3$	58.98978	96.72	+1041
$^{178}Hf^{3}$	59.3143	27.14	
$^{119}Sn^{2}$	59.45158	08.58	
$^{179}Hf^{3}$	59.6484	13.75	
^{60}Ni	59.93077	26.23	-----
^{59}CoH	59.94100	99.985	+5858
$^{30}Si_2$	59.94752	00.10	+3578
^{60}TiC	59.94795	73.24	+3488
^{28}SiS	59.94900	87.60	+3287
^{44}CaO	59.95041	02.06	+3051
$^{135}Ba^{43}$	59.95082	06.59	+2889
$^{120}Sn^{2}$	59.95110	32.58	+2948
^{120}Te	59.95225	00.089	+2790
^{48}CaC	59.95253	00.183	+2754
$^{28}SiO_2$	59.96676	91.77	+1665
$^{36}SC_2$	59.96709	00.013	+1650
$^{24}Mg_2C$	59.97008	60.57	+1525
$^{180}W^{3}$	59.9815	00.135	+1181
$^{180}Ta^{3}$	59.982/	00.012	+1170
$^{180}Hf^{3}$	59.9820	35.24	+1170
$^{12}CO_3$	59.98473	98.18	+1111
$^{24}MgC_3$	59.98504	76.12	+1105
$^{60}C_5$	60.00000	94.57	+ 866
$^{181}Ta^{3}$	60.3153	99.988	
$^{136}Ba^{43}$	60.40194	07.81	
$^{121}Sb^{2}$	60.45186	57.25	
$^{182}W^{3}$	60.6487	26.41	
$^{137}Ba^{43}$	60.84692	11.32	
^{61}Ni	60.93109	01.19	-----
^{60}NiH	60.93859	26.23	+8124
^{61}TiC	60.94787	05.27	+3631
^{45}ScO	60.95083	99.76	+3087
$^{122}Te^{2}$	60.95145	04.72	+2993
$^{122}Sn^{2}$	60.95173	04.72	+2952
$^{37}ClC_2$	60.96590	23.93	+1750
$^{29}SiO_2$	60.96632	04.68	+1730
$^{61}Mg_2C$	60.97088	16.29	+1531
$^{188}W^{3}$	60.9827	14.40	+1180
$^{13}CO_3$	60.98809	01.10	+1069
$^{61}MgC_3$	60.98584	12.48	+1114
$^{61}C_5$	61.00336	05.30	+ 843
$^{12}C_5H$	61.00782	94.56	+ 794
$^{138}Ba^{43}$	61.29106	71.66	-2429
$^{184}Os^{3}$	61.315/	00.018	-47E3
$^{184}W^{3}$	61.3163	30.64	-----
$^{123}Sb^{2}$	61.45209	42.75	-----
$^{123}Te^{2}$	61.4522	00.87	+56E4
$^{185}Re^{3}$	61.649/	37.07	+ 312
$^{139}La^{43}$	61.73601	99.911	
^{62}Ni	61.92834	03.66	-----
^{61}NiH	61.93891	01.19	+5859
^{50}CrC	61.94065	04.26	+5031
^{62}TiC	61.94479	05.34	+3765
^{50}VC	61.94716	00.24	+3291
$^{31}P_2$	61.94753	100.00	+3227
^{46}CaO	61.94754	3.3E3	+3225
^{46}TiO	61.94854	07.27	+3066

$^{124}Te^{2}$	61.95156	04.61	+2667
$^{124}Sn^{2}$	61.95262	05.94	+2551
$^{124}Xe^{2}$	61.95306	00.096	+2505
$^{30}SiO_2$	61.96359	03.07	+1757
$^{62}Mg_2C$	61.96763	18.19	+1576
$^{23}Na_2O$	61.97447	99.76	+1343
$^{62}MgC_3$	61.98259	11.25	+1141
$^{186}W^{3}$	61.9836	28.41	+1121
$^{186}Os^{3}$	61.984	01.59	+1113
$^{14}NO_3$	61.98780	98.91	+1042
$^{62}C_5$	62.00670	00.119	+ 790
$^{12}C_5H_2$	62.01564	94.55	+ 709
$^{140}Ce^{43}$	62.18012	88.48	
$^{187}Re^{3}$	62.318/	62.93	-----
$^{187}Os^{3}$	62.319/	01.64	+62E3
$^{125}Te^{2}$	62.45231	06.99	
$^{188}Os^{3}$	62.6523	13.3	
^{63}Cu	62.92959	69.09	-----
^{62}NiH	62.93616	03.66	+9578
^{51}VC	62.94398	98.66	+4373
^{47}TiO	62.94667	07.26	+3684
$^{50}Ti^{13}C$	62.94814	00.059	+3392
$^{50}Cr^{13}C$	62.94940	00.048	+3177
$^{126}Te^{2}$	62.95194	18.71	+2816
$^{126}Xe^{2}$	62.95223	00.09	+2780
$^{31}PO_2$	62.96358	99.52	+1850
$^{39}KC_2$	62.96371	91.05	+1844
$^{27}AlC_3$	62.98154	96.72	+1212
$^{189}Os^{3}$	62.9862/	16.1	+1112
$^{63}C_5$	63.01008	01.3E3	+ 782
C_5H_3	63.02346	94.55	+ 670
$^{190}Os^{3}$	63.3183	26.4	-----
$^{190}Pt^{3}$	63.321/	00.013	+24E3
$^{127}I^{2}$	63.45233	100.00	
$^{191}Ir^{3}$	63.6545	37.3	-2157
$^{85}Rb^{32}$	63.68402	72.15	-----
^{64}Ni	63.92796	01.08	-54E3
^{64}Zn	63.92914	48.89	-----
^{63}CuH	63.93741	69.08	+7730
^{52}CrC	63.94051	82.83	+5623
^{48}TiO	63.94286	73.76	+4660
$^{32}S_2$	63.94414	90.25	+4262
^{48}CaO	63.94744	00.185	+3493
$^{24}Mg^{40}Ca$	63.94790	76.32	+3408
$^{128}Xe^{2}$	63.95176	01.919	+2826
$^{46}Ti^{18}O$	63.95179	00.016	+2821
$^{128}Te^{2}$	63.95278	31.79	+2704
$^{32}SO_2$	63.96190	94.54	+1951
$^{40}CaC_2$	63.96259	94.83	+1911
$^{64}KC_2$	63.96706	02.05	+1686
$^{24}Mg_2O$	63.96499	61.79	+1783
$^{28}SiC_3$	63.97693	89.18	+1339
$^{192}Os^{3}$	63.9874	41.0	+1097
$^{192}Pt^{3}$	63.9883	00.78	+1081
$^{12}C_4O$	63.99491	95.41	+ 972
C_5H_4	64.03128	94.52	+ 626
$^{193}Ir^{3}$	64.3222	62.7	
$^{129}Xe^{2}$	64.45237	26.44	
$^{194}Pt^{3}$	64.6544/	32.9	
^{65}Cu	64.92778	30.91	-----
^{64}NiH	64.93578	01.08	+8116
^{64}ZnH	64.93696	48.88	+7072
^{53}CrC	64.94065	09.44	+5045
^{49}TiO	64.94278	05.50	+4329
$^{65}S_2$	64.94354	01.44	+4120
$^{52}Cr^{13}C$	64.94386	00.927	+4038
$^{47}Ti^{18}O$	64.95092	00.015	+2808
$^{130}Xe^{2}$	64.95175	04.08	+2709
$^{130}Ba^{2}$	64.95312	00.101	+2562
$^{130}Te^{2}$	64.95348	34.48	+2526
$^{41}KC_2$	64.96183	06.73	+1907
$^{49}Mg_2O$	64.96597	15.91	+1700
$^{65}SiC_3$	64.97649	07.55	+1333
$^{195}Pt^{3}$	64.9887	33.8	+1066
C_5H_5	65.03910	94.51	+ 583
$^{196}Hg^{3}$	65.32194	00.146	-13E4
$^{196}Pt^{3}$	65.3224	25.3	-----
$^{131}Xe^{2}$	65.45354	21.18	
$^{197}Au^{3}$	65.6557	100.00	
^{66}Zn	65.92605	27.81	-----
$^{88}Sr^{32}$	65.92951	82.56	+19E3
^{65}CuH	65.93560	30.91	+6903
^{54}CrC	65.93887	02.35	+5142
^{54}FeC	65.93961	05.76	+4862
^{50}TiO	65.93970	05.32	+4829
$^{66}S_2$	65.93993	08.02	+4750
^{50}CrO	65.94096	04.30	+4422

^{50}VO	65.94207	00.24	+4115
$^{33}S_2$	65.94293	00.006	+3906
$^{53}Cr^{13}C$	65.94401	00.106	+3673
^{39}KAl	65.94525	93.10	+3434
$^{48}Ti^{18}O$	65.94711	00.151	+3132
$^{132}Xe^2$	65.95208	26.89	+2533
$^{132}Ba^2$	65.95256	00.097	+2487
$^{34}SO_2$	65.95769	04.20	+2024
$^{50}Mg_2O$	65.96254	18.53	+1809
$^{25}Mg_2O$	65.96659	01.03	+1626
$^{27}Al_2C$	65.96308	98.90	+1780
$^{66}SiC_3$	65.97376	03.14	+1381
$^{198}Pt^3$	65.9738	07.21	+1381
$^{198}Hg^3$	65.98392	10.02	+1049
$^{12}C^2_{11}$	66.00000	88.45	+ 891
C_5H_6	66.04692	94.50	+ 545
$^{199}Hg^3$	66.32274	16.84	
$^{133}Cs^2$	66.45257	100.00	-----
$^{133}C^2_{11}$	66.50168	10.90	+1353
$^{200}Hg^3$	66.65611	23.13	-----
$^{89}Y^{32}$	66.67929	100.00	+2876
^{67}Zn	66.92714	04.11	-----
^{66}ZnH	66.93387	27.81	+9945
^{55}MnC	66.93805	98.89	+6134
^{51}VO	66.93889	99.52	+5696
$^{67}S_2$	66.93933	00.064	+5490
$^{28}Si^{39}K$	66.94064	85.85	+4958
$^{54}Cr^{13}C$	66.94222	00.026	+4438
$^{54}Fe^{13}C$	66.94296	00.064	+4231
$^{40}Ca^{27}Al$	66.94440	96.97	+3878
$^{49}Ti^{18}O$	66.94711	00.011	+3370
$^{134}Ba^2$	66.95213	02.42	+2678
$^{134}Xe^2$	66.95271	10.44	+2617
$^{35}ClO_2$	66.95865	75.17	+2124
$^{67}CaC_2$	66.95878	00.157	+2115
$^{31}PC_3$	66.97376	96.72	+1434
$^{201}Hg^3$	66.99010	13.22	+1063
$^{134}C^2_{11}$	67.00336	00.611	+ 878
C_5H_7	67.05474	94.49	+ 525
$^{202}Hg^3$	67.32354	29.80	
$^{135}Ba^2$	67.45278	06.59	
$^{90}Zr^{32}$	67.42825	51.46	
$^{203}Tl^3$	67.6573	29.50	
^{68}Zn	67.92486	18.57	-----
^{56}FeC	67.93194	90.64	+9594
^{67}ZnH	67.93496	04.11	+6725
^{52}CrO	67.93543	83.56	+6426
$^{68}S_2$	67.93573	00.204	+6249
$^{28}SiCa$	67.93979	89.42	+4550
$^{55}Mn^{13}C$	67.94140	01.107	+4107
^{41}KAl	67.94337	06.88	+3670
$^{50}Ti^{18}O$	67.94395	00.011	+3558
$^{50}Cr^{18}O$	67.94521	00.009	+3339
$^{136}Ba^2$	67.95219	07.81	+2485
$^{136}Ce^2$	67.95354	00.193	+2365
$^{136}Xe^2$	67.95360	08.87	+2363
$^{28}Si_2C$	67.95386	84.09	+2342
$^{44}CaC_2$	67.95500	02.015	+2254
$^{32}SC_3$	67.97207	91.88	+1439
$^{204}Pb^3$	67.99103	01.48	+1027
$^{204}Hg^3$	67.99116	06.85	+1025
C_5H_8	68.06256	94.43	+ 493
$^{205}Tl^3$	68.3246	70.50	
$^{137}Ba^2$	68.45279	11.32	
$^{206}Pb^3$	68.65815	23.6	
^{69}Ga	68.92571	60.4	-----
$^{92}Zr^{32}$	68.92850	17.11	+25E3
^{68}ZnH	68.93268	18.57	+9889
$^{56}Fe^{13}C$	68.93529	01.015	+7194
^{57}FeC	68.93541	02.166	+7106
^{53}CrO	68.93556	09.53	+6998
$^{69}S_2$	68.93855	02.E4	+5368
$^{138}Ba^2$	68.95244	71.66	+2579
$^{138}Ce^2$	68.95302	00.25	+2524
$^{138}La^2$	68.95337	00.089	+2487
$^{69}Si_2C$	68.95342	09.50	+2487
$^{37}ClO_2$	68.95570	24.35	+2298
$^{45}ScC_2$	68.95592	97.80	+2282
$^{69}SC_3$	68.97542	03.83	+1387
$^{207}Pb^3$	68.99196	22.6	+1040
C_5H_9	69.0704	94.46	+ 476
$^{208}Pb^3$	69.32555	52.3	
$^{139}La^2$	69.45302	99.911	
$^{209}Bi^3$	69.65978	100.00	
^{70}Ge	69.92399	20.52	-----
^{70}Ge	69.92399	20.52	-----
^{70}Zn	69.92534	00.62	+52E3
^{70}FeC	69.93331	00.35	+7503
^{69}GaH	69.93353	60.4	+7330
^{54}CrO	69.93379	02.38	+7135
^{54}FeO	69.93452	05.81	+6640
$^{70}S_2$	69.93495	00.001	+6380
^{58}NiC	69.93535	68.41	+6155
$^{35}Cl_2$	69.93771	56.05	+5097
$^{57}Fe^{13}C$	69.93876	00.024	+4734
$^{52}Cr^{18}O$	69.93967	00.171	+4451
$^{70}Si_2C$	69.95069	05.95	+2619
$^{46}CaC_2$	69.95369	00.003	+2354
$^{46}TiC_2$	69.95263	07.82	+2442
$^{27}Al_2O$	69.95799	99.76	+2058
$^{70}SC_3$	69.96786	04.10	+1592
C_5H_{10}	70.0782	94.45	+ 453
Na_2C_2	69.97976	97.80	+1254
$^{94}Zr^{32}$	70.43073	17.40	-----
$^{141}Pr^2$	70.45374	100.00	+3062
^{71}Ga	70.92482	39.6	-----
^{70}GeH	70.93181	20.52	+10E3
^{55}MnO	70.93297	99.76	+8702
^{59}CoC	70.93318	98.89	+8484
$^{44}CaAl$	70.93654	02.06	+6052
$^{58}Fe^{13}C$	70.93666	03.7E3	+5990
$^{58}Ni^{13}C$	70.93870	00.766	+5110
$^{53}Cr^{18}O$	70.93981	00.019	+4735
$^{54}FeOH$	70.94231	05.81	+4055
$^{71}TiC_2$	70.95176	07.31	+2633
$^{39}KO_2$	70.95351	92.65	+2472
$^{142}Nd^2$	70.95374	27.11	+2452
$^{142}Ce^2$	70.95465	11.07	+2378
$^{23}NaO_3$	70.97451	96.72	+1427
$^{23}NaC_4$	70.98978	95.65	+1091
C_5H_{11}	71.08602	94.44	+ 440
$^{143}Nd^2$	71.45479	12.17	
^{72}Ge	71.92159	27.43	-----
^{56}FeO	71.92685	91.44	+14E3
^{60}NiC	71.93077	25.94	+7835
$^{72}SiCa$	71.93193	01.93	+6956
^{71}GaH	71.93264	39.6	+6509
$^{36}S_2$	71.93418	3.0E6	+5713
$^{72}Cl_2$	71.93476	36.97	+5461
$^{59}Co^{13}C$	71.93653	01.107	+4814
$^{54}Cr^{18}O$	71.93803	00.005	+4383
$^{54}Fe^{18}O$	71.93877	00.012	+4179
$^{72}TiC_2$	71.94795	72.50	+2728
$^{29}Si_2O$	71.94877	34.33	+2646
$^{40}CaO_2$	71.95239	96.50	+2335
$^{48}CaC_2$	71.95253	00.181	+2325
$^{144}Nd^2$	71.95490	23.85	+2159
$^{24}Mg_3$	71.95513	[illegible]	+2145
$^{144}Sm^2$	71.95583	03.09	+2101
$^{24}MgO_3$	71.96977	78.13	+1493
$^{24}Mg_2C_2$	71.97008	60.58	+1483
$^{24}MgC_4$	71.98504	75.27	+1134
$^{72}C_6$	72.00000	93.52	+ 917
$^{145}Nd^2$	72.45603	08.30	-----
$^{145}C^2_{12}$	72.50168	11.76	+1587
^{73}Ge	72.92334	07.76	-----
^{72}GeH	72.92941	27.43	+12E3
^{57}FeO	72.93032	02.19	+10E3
^{73}NiC	72.93109	01.47	+9409
$^{56}FeOH$	72.93464	91.45	+6453
$^{55}Mn^{18}O$	72.93721	00.204	+5261
$^{73}TiC_2$	72.94787	07.01	+2973
$^{73}Si_2O$	72.94833	08.64	+2919
$^{41}KO_2$	72.95163	06.85	+2578
$^{73}Mg_3$	72.95592	18.32	+2238
$^{146}Nd^2$	72.95635	17.22	+2209
$^{37}ClC_3$	72.96590	23.67	+1713
$^{25}MgO_3$	72.97057	10.06	+1544
$^{73}Mg_2C_2$	72.97088	16.96	+1534
$^{73}MgC_4$	72.98584	13.07	+1167
$^{73}C_6$	73.00336	06.29	+ 911
$^{12}C_6H$	73.00782	93.51	+ 863
$^{147}Sm^2$	73.45725	14.97	
^{74}Ge	73.92100	36.54	-----
^{74}Se	73.92254	00.87	+48E3
^{58}FeO	73.92822	00.33	+10E3
^{74}NiC	73.92834	03.63	+10E3
^{58}NiO	73.93026	69.01	+7983
$^{56}Fe^{18}O$	73.93110	00.187	+7319
^{73}GeH	73.93116	07.76	+7276
$^{37}Cl_2$	73.93181	05.99	+6838
^{39}KCl	73.93256	70.32	+6395
$^{57}FeOH$	73.93814	02.18	+4323
$^{50}CrC_2$	73.94065	04.22	+3762
$^{74}TiC_2$	73.94479	05.34	+3107
$^{58}Si_2O$	73.94560	05.91	+3005
$^{42}CaO_2$	73.94843	00.64	+2695
$^{74}Mg_3$	73.95268	23.18	+2333
$^{148}Sm^2$	73.95721	11.24	+2041
$^{148}Nd^2$	73.95823	05.73	+1986
$^{26}MgO_3$	73.96732	11.09	+1597
$^{74}Mg_2C_2$	73.96763	18.54	+1585
$^{74}MgC_4$	73.98259	11.11	+1200
$^{74}C_6$	74.00670	00.176	+ 863
$^{12}C_6H_2$	74.01564	93.50	+ 781
$^{149}Sm^2$	74.45840	13.83	
^{75}As	74.92171	100.00	-----
^{59}CoO	74.92809	99.76	+12E3
^{74}GeH	74.92882	36.53	+11E3
$^{48}TiAl$	74.92949	73.98	+9630
^{63}CuC	74.92959	68.33	+9506
^{74}SeH	74.93036	00.87	+8661
$^{57}Fe^{18}O$	74.93457	00.004	+5812
$^{51}VC_2$	74.94398	97.56	+3364
$^{75}Mg_3$	74.95347	05.34	+2359
$^{25}Mg_3$	74.95752	00.01	+2092
$^{150}Sm^2$	74.95845	07.44	+2039
$^{43}CaO_2$	74.95858	00.145	+2032
$^{150}Nd^2$	74.96041	05.63	+1936
$^{39}KC_3$	74.96371	90.04	+1784
$^{27}AlO_3$	74.96627	99.28	+1681
$^{27}AlC_4$	74.98154	95.65	+1253
C_6H_3	75.02346	93.48	+ 736
$^{151}Eu^2$	75.45977	47.32	
^{76}Se	75.91928	09.02	-----
^{76}Ge	75.92019	07.76	+38E3
^{60}NiO	75.92568	26.17	+12E3
^{64}NiC	75.92796	01.07	+8746
^{64}ZnC	75.92914	48.35	+7700
^{75}AsH	75.92953	99.985	+7407
^{76}KCl	75.92961	27.98	+7349
$^{63}Cu^{13}C$	75.93292	00.765	+5566
$^{52}CrC_2$	75.94051	81.92	+3576
$^{32}S_2C$	75.94414	89.25	+3054
$^{44}CaO_2$	75.94529	02.05	+2919
$^{76}Mg_3$	75.95023	03.29	+2453
$^{152}Sm^2$	75.95968	26.72	+1879
$^{152}Gd^2$	75.95971	00.20	+1878
$^{28}SiO_3$	75.96166	91.54	+1791
$^{40}CaC_3$	75.96259	93.79	+1753
$^{28}SiC_4$	75.97693	88.19	+1318
$^{12}CO_4$	75.97964	97.84	+1259
$^{12}C_6H_4$	76.03123	93.47	+ 678
$^{153}Eu^2$	76.4603	52.18	
^{77}Se	76.91998	07.58	-----
^{61}NiO	76.92600	01.19	+13E3
^{76}SeH	76.92710	09.02	+11E3
^{65}CuC	76.92778	30.57	+9862
^{76}GeH	76.92801	07.76	+9579
^{65}CuC	76.92778	30.57	+9862
$^{64}Zn^{13}C$	76.93131	00.54	+6789
$^{53}CrC_2$	76.94065	09.34	+3721
$^{52}Cr^{13}C_2$	76.94387	01.33	+3220
$^{45}ScO_2$	76.94752	99.52	+2793
$^{77}Mg_3$	76.95102	00.38	+2478
$^{154}Gd^2$	76.96047	02.15	+1900
$^{154}Sm^2$	76.96097	22.71	+1877
$^{29}SiO_3$	76.96122	04.67	+1865
$^{41}KC_3$	76.96183	06.65	+1833
$^{77}SiC_4$	76.97649	08.46	+1361
$^{13}CO_4$	76.98300	01.10	+1221
$^{12}C_6H_5$	77.03910	93.46	+ 646
$^{232}Th^3$	77.3460	100.00	
$^{155}Gd^2$	77.4614	14.73	
^{78}Se	77.91739	23.52	-----
^{78}Kr	77.92019	00.354	+28E3
^{62}NiO	77.92325	03.64	+13E3
^{66}ZnC	77.92605	27.50	+8997
$^{39}K_2$	77.92742	86.68	+7768
$^{41}K^{37}Cl$	77.92773	01.68	+7536
^{77}SeH	77.92780	07.58	+7485
$^{65}Cu^{13}C$	77.93113	00.34	+5671
$^{78}CrC_2$	77.93887	02.54	+3627
$^{54}FeC_2$	77.93961	05.69	+3507
$^{78}S_2C$	77.93993	07.95	+3457
$^{46}TiO_2$	77.94243	07.96	+3112
$^{78}Mg_3$	77.94777	00.14	+2566
$^{156}Dy^2$	77.957/	00.052	+1967

$^{30}SiO_3$	77.95849	03.07	+1895
$^{42}CaC_3$	77.95863	00.62	+1889
$^{156}Gd^{2}$	77.96113	20.47	+1781
$^{31}P_2O$	77.96244	99.76	+1730
$^{27}Al_2C_2$	77.96308	97.80	+1705
$^{23}Na_2O_2$	77.96938	97.52	+1499
$^{78}SiC_4$	77.97376	03.16	+1382
$^{14}NO_4$	77.98271	98.67	+1193
$^{12}C^{2}_{13}$	78.00000	86.49	+ 943
$^{12}C_6H_6$	78.04692	93.45	+ 602
$^{235}U^{3}$	78.3476	00.72	
$^{157}Gd^{2}$	78.4621	15.68	-----
$^{157}C^{2}_{13}$	78.50168	12.60	+1982
^{79}Br	78.91839	50.537	-----
$^{52}CrAl$	78.92205	83.76	+22E3
^{63}CuO	78.92451	68.92	+13E3
^{78}SeH	78.92521	23.52	+12E3
^{79}ZnC	78.92714	04.42	+9019
$^{79}K_2$	78.92771	00.022	+8468
$^{66}Zn^{13}C$	78.92941	00.31	+7168
$^{55}MnC_2$	78.93805	97.80	+4014
$^{47}TiO_2$	78.94156	07.25	+3406
$^{31}PO_3$	78.95849	99.28	+1968
$^{79}CaC_3$	78.95878	00.161	+1954
$^{158}Dy^{2}$	78.96200	00.09	+1810
$^{158}Gd^{2}$	78.9622	24.87	+1801
$^{31}PC_4$	78.97376	95.65	+1425
$^{158}C^{2}_{13}$	79.00335	00.847	+ 929
C_6H_7	79.05474	93.44	+ 579
$^{238}U^{3}$	79.3495	99.274	-----
$^{159}Tb^{2}$	79.46244	100.000	+ 703
^{80}Se	79.91647	49.82	-----
^{80}Kr	79.91659	02.27	+67E4
$^{28}Si^{52}Cr$	79.91744	77.24	+82E3
^{64}NiO	79.92287	01.08	+13E3
^{64}ZnO	79.92405	48.77	+11E3
^{80}ZnC	79.92486	18.41	+9525
$^{40}Ca_2$	79.92517	93.45	+9186
$^{80}K_2$	79.92554	12.81	+8811
$H^{79}Br$	79.92622	50.52	+8197
$^{56}FeC_2$	79.93194	89.64	+5166
$^{55}Mn^{25}C_2$	79.94141	02.19	+3204
$^{48}TiO_2$	79.93775	73.62	+3755
$^{32}S_2O$	79.93905	90.03	+3539
$^{48}CaO_2$	79.94233	00.184	+3090
$^{28}Si_2C_2$	79.95386	83.16	+2137
$^{44}CaC_3$	79.95500	01.99	+2074
$^{32}SO_3$	79.95602	94.32	+1981
$^{24}Mg_2O_2$	79.95990	61.64	+1840
$^{160}Dy^{2}$	79.9620	02.294	+1755
$^{160}Gd^{2}$	79.96361	21.90	+1695
$^{32}SC_4$	79.97207	92.77	+1437
$^{12}C_6H_8$	80.06256	93.43	+ 547
$^{161}Dy^{2}$	80.4629	18.88	
^{81}Br	80.91642	49.463	-----
$^{54}FeAl$	80.92115	05.82	+17E3
^{65}CuO	80.92269	30.84	+13E3
^{80}SeH	80.92429	49.81	+10E3
^{69}GaC	80.92571	59.73	+8710
$^{81}FeC_2$	80.93541	04.15	+4261
$^{49}TiO_2$	80.93767	05.48	+3808
$^{27}Al_3$	80.94462	100.00	+2869
$^{81}Si_2C_2$	80.95342	12.12	+2187
$^{49}Mg_2O_2$	80.96070	15.87	+1827
$^{162}Dy^{2}$	80.9628	25.53	+1745
$^{162}Er^{2}$	80.96436	00.136	+1688
$^{12}C_6H_9$	81.07038	93.41	+ 526
$^{163}Dy^{2}$	81.4639	24.97	
^{82}Kr	81.91345	11.56	-26E3
$^{28}Si^{54}Fe$	81.91654	05.37	-91E4
^{82}Se	81.91663	09.19	-----
$^{55}MnAl$	81.91959	100.00	+28E3
^{66}ZnO	81.92096	27.74	+19E3
$^{82}Ca_2$	81.92121	01.24	+18E3
$^{41}K_2$	81.92366	00.47	+12E3
^{70}GeC	81.92399	20.29	+11E3
$H^{81}Br$	81.92425	49.44	+11E3
^{70}ZnC	81.92534	00.63	+9405
$^{69}Ga^{13}C$	81.92906	00.669	+6590
$^{82}FeC_2$	81.93331	00.368	+4911
$^{50}TiO_2$	81.93459	05.31	+4561
$^{58}NiC_2$	81.93535	67.66	+4376
$^{66}S_2O$	81.93484	08.00	+4498
$^{50}CrO_2$	81.93585	04.29	+4262
$^{82}Si_2C_2$	81.95069	05.98	+2405
$^{34}SO_3$	81.95261	04.19	+2277
$^{46}TiC_3$	81.95263	07.74	+2275
$^{50}Mg_2O_2$	81.95745	18.53	+2007
$^{164}Dy^{2}$	81.9643	28.18	+1718
$^{164}Er^{2}$	81.9649	01.56	+1697
$^{34}SC_4$	81.96786	04.04	+1599
$^{165}Ho^{2}$	82.46455	100.00	
$^{56}FeAl$	82.91348	91.66	-15E4
^{83}Kr	82.91405	11.55	-----
$^{28}Si^{55}Mn$	82.91498	92.21	+89E3
^{67}ZnO	82.92205	04.10	+10E3
$^{83}Ca_2$	82.92278	00.28	+9498
^{82}SeH	82.92445	09.19	+7973
^{71}GaC	82.92482	39.16	+7699
$^{59}CoC_2$	82.93318	97.80	+4334
$^{51}VO_2$	82.93378	99.28	+4202
$^{83}TiC_3$	82.95176	07.31	+2199
$^{35}ClO_3$	82.95355	74.98	+2099
$^{166}Er^{2}$	82.9644	33.41	+1647
$^{35}ClC_4$	82.96885	72.24	+1513
$^{167}Er^{2}$	83.4653	22.94	
$^{28}Si^{56}Fe$	83.90887	84.52	-19E3
^{84}Kr	83.91325	56.90	-48E3
^{84}Sr	83.91325	00.56	-----
$^{57}FeAl$	83.91695	02.19	+23E3
$^{84}Ca_2$	83.91808	03.98	+17E3
^{68}ZnO	83.91977	18.53	+13E3
^{72}GeC	83.92159	27.13	+10E3
$^{52}CrO_2$	83.93031	83.36	+4919
$^{28}Si_3$	83.93079	78.40	+4784
$^{60}NiC_2$	83.93078	25.65	+4787
$^{84}TiC_3$	83.94795	71.79	+2418
$^{48}CaC_3$	83.95253	00.18	+2136
$^{168}Er^{2}$	83.9654	27.07	+1609
$^{168}Yb^{2}$	83.96695	00.135	+1563
$^{12}C_7$	84.00000	92.48	+ 967
$^{169}Tm^{2}$	84.46717	100.00	-----
$^{169}C^{2}_{14}$	84.50168	13.42	+2448
$^{85}SiFe$	84.90843	06.33	-24E3
^{85}Rb	84.91202	72.15	-----
$^{58}FeAl$	84.91485	00.33	+30E3
^{84}SrH	84.92107	00.56	+9383
^{85}GeC	84.92334	07.97	+7501
$^{85}Si_3$	84.93035	11.99	+4632
$^{53}CrO_2$	84.93045	09.50	+4607
$^{85}NiC_2$	84.93109	01.73	+4453
$^{85}TiC_3$	84.94787	07.73	+2369
$^{37}ClC_4$	84.96590	02.40	+1576
$^{170}Yb^{2}$	84.967/	03.03	+1544
$^{170}Er^{2}$	84.9678	14.88	+1522
$^{85}C_7$	85.00336	07.25	+ 930
$^{12}C_7H$	85.00782	92.49	+ 886
$^{171}Yb^{2}$	85.468/	14.31	
^{86}Sr	85.90935	09.86	-----
^{86}Kr	85.91079	17.37	+60E3
$^{54}Fe^{32}S$	85.91168	05.53	+37E3
^{70}GeO	85.91390	60.3	+8996
^{85}RbH	85.91984	72.14	+8190
^{70}ZnO	85.92025	00.62	+7382
^{86}GeC	85.92100	36.23	+7374
^{74}SeC	85.92254	00.87	+6513
$^{86}Si_3$	85.92762	08.49	+4702
$^{62}NiC_2$	85.92834	03.58	+4524
$^{54}CrO_2$	85.92867	02.37	+4446
$^{54}FeO_2$	85.92941	05.79	+4283
$^{86}TiC_3$	85.94479	05.34	+2424
$^{50}CrC_3$	85.94065	04.17	+2341
$^{27}Al_2O_2$	85.95289	99.52	+1973
$^{172}Yb^{2}$	85.9626	21.82	+1612
$^{31}P_2C_2$	85.96753	97.80	+1477
$^{86}C_7$	86.00670	00.244	+ 882
$^{12}C_7H_2$	86.01564	92.48	+ 808
$^{173}Yb^{2}$	86.469/	16.13	
^{87}Sr	86.90899	07.02	-----
^{87}Rb	86.90930	27.85	+28E4
^{86}SrH	86.91717	09.86	+11E3
^{71}GaO	86.91973	39.50	+8092
^{75}AsC	86.92171	98.89	+6832
$^{74}Ge^{13}C$	86.92436	00.40	+5654
$^{55}MnO_2$	86.92785	99.52	+4608
$^{87}Si_3$	86.92718	00.81	+4773
$^{39}KO_3$	86.94841	92.43	+2205
$^{174}Yb^{2}$	86.9628/	31.84	+1615
$^{39}KC_4$	86.96371	89.05	+1588
$^{174}Hf^{2}$	86.970/	00.18	+1425
$^{12}C_7H_3$	87.02346	92.47	+ 759
$^{175}Lu^{2}$	87.471/	97.41	
$^{56}Fe^{32}S$	87.90401	87.08	-44E3
^{88}Sr	87.90601	82.56	-----
$^{40}Ca^{48}Ti$	87.91081	71.74	+18E3
^{72}GeO	87.91650	27.37	+8372
$^{88}Ca_2$	87.91653	00.40	+8348
^{87}SrH	87.91681	07.02	+8139
^{87}RbH	87.91712	27.85	+7912
^{76}SeC	87.91928	08.92	+6624
^{76}GeC	87.92129	07.67	+5753
$^{56}FeO_2$	87.92174	91.22	+5585
$^{88}Si_3$	87.92445	00.28	+4767
$^{64}ZnC_2$	87.92914	47.81	+3801
$^{64}NiC_2$	87.92796	01.06	+4003
$^{52}CrC_3$	87.94051	81.01	+2547
$^{28}Si_2O_2$	87.94368	84.62	+2333
$^{32}S_2C_2$	87.94414	88.26	+2305
$^{40}CaO_3$	87.94759	96.27	+2114
$^{40}CaC_4$	87.96286	92.75	+1546
$^{24}MgO_4$	87.96468	77.94	+1498
$^{176}Hf^{2}$	87.9704	05.20	+1365
$^{176}Lu^{2}$	87.9710	02.59	+1352
$^{176}Yb^{2}$	87.97136	12.73	+1345
$^{12}C_7H_4$	88.03128	92.46	+ 702
$^{177}Hf^{2}$	88.4713	18.50	
^{89}Y	88.90572	100.00	-----
$^{57}Fe^{32}S$	88.90748	02.08	+51E3
^{88}SrH	88.91383	82.55	+11E3
^{73}GeO	88.91825	07.73	+7095
^{89}SeC	88.91998	07.60	+6235
$^{89}Si_3$	88.92401	00.013	+4861
$^{57}FeO_2$	88.92521	02.18	+4562
$^{65}CuC_2$	88.92778	30.23	+4030
$^{89}CrC_3$	88.94065	11.96	+2545
$^{89}Si_2O_2$	88.94324	08.62	+2370
$^{41}KO_3$	88.94563	06.83	+2228
$^{41}KC_4$	88.96183	06.58	+1584
$^{25}MgO_4$	88.96548	10.03	+1488
$^{178}Hf^{2}$	88.9715	27.14	+1352
$^{12}C_7H_5$	89.03910	92.45	+ 667
$^{179}Hf^{2}$	89.4726	13.75	
^{90}Zr	89.90433	51.46	-----
$^{45}Sc_2$	89.91184	100.00	+12E3
^{89}YH	89.91354	99.985	+9762
^{74}GeO	89.91591	36.38	+7764
^{90}SeC	89.91739	23.32	+6884
^{74}SeO	89.91745	00.87	+6852
$^{58}FeO_2$	89.92311	00.32	+4787
$^{58}NiO_2$	89.92515	68.85	+4318
$^{66}ZnC_2$	89.92605	27.20	+4139
$^{39}K_2C$	89.92742	85.72	+3894
$^{90}CrC_3$	89.93887	02.61	+2602
$^{54}FeC_3$	89.93961	05.63	+2548
$^{90}Si_2O_2$	89.94051	05.89	+2485
$^{26}MgO_4$	89.96223	11.06	+1553
$^{27}Al_2C_3$	89.96308	96.72	+1530
$^{180}W^{2}$	89.9723	00.135	+1323
$^{180}Ta^{2}$	89.973/	00.012	+1309
$^{180}Hf^{2}$	89.9731	35.24	+1307
$^{12}C^{2}_{15}$	90.00000	84.58	+ 940
$^{12}C_7H_6$	90.04692	92.43	+ 631
$^{181}Ta^{2}$	90.4729	99.988	-----
$^{181}C^{2}_{15}$	90.50168	14.22	+3144
^{91}Zr	90.90532	11.22	-----
^{90}ZrH	90.91215	51.45	+13E3
^{75}AsO	90.91662	99.76	+8045
^{79}BrC	90.91839	49.98	+6955
$^{59}CoC_2$	90.92298	97.80	+5148
$^{91}ZnC_2$	90.92714	04.63	+4166
$^{55}MnC_3$	90.93805	96.72	+2777
$^{54}Fe^{37}C_3$	90.94297	00.189	+2414
$^{27}AlO_4$	90.96114	99.04	+1629
$^{182}W^{2}$	90.9730	26.41	+1343
$^{182}C^{2}_{15}$	91.00335	01.115	+ 927
$^{183}W^{2}$	91.4741	14.40	
$^{40}Ca^{52}Cr$	91.90337	81.22	-71E3
^{92}Zr	91.90467	17.11	-----
$^{46}Ti_2$	91.90526	00.64	+16E4
^{92}Mo	91.90855	15.84	+24E3
^{91}ZrH	91.91314	11.22	+11E3
^{76}SeO	91.91419	09.01	+9654
^{76}GeO	91.91620	07.75	+7971
^{80}SeC	91.91647	49.27	+7789
$^{60}NiO_2$	91.92057	26.10	+5780
$^{92}ZnC_2$	91.92486	18.25	+4552

$^{40}Ca_{2}C$	91.92517	92.42	+4483
$^{44}CaO_{3}$	91.94023	02.05	+2584
$^{28}Si_{2}C_{3}$	91.95386	82.24	+1868
$^{44}CaC_{4}$	91.95550	01.97	+1808
$^{28}SiO_{4}$	91.95657	91.32	+1771
$^{184}Os^{2}$	91.973	00.018	+1345
$^{184}W^{2}$	91.9745	30.64	+1316
$^{185}Re^{2}$	92.474	37.07	
^{93}Nb	92.90566	100.00	-----
^{92}ZrH	92.91249	17.11	+14E3
^{77}SeO	92.91489	07.57	+10E3
^{81}BrC	92.91642	48.92	+8634
$^{61}NiO_{2}$	92.92089	01.18	+6100
$^{69}GaC_{2}$	92.92571	59.07	+4634
$^{93}FeC_{3}$	92.93530	05.10	+3134
$^{27}Al_{3}C$	92.94462	98.89	+2385
$^{31}P_{3}$	92.95129	100.00	+2036
$^{93}Si_{2}C_{3}$	92.95342	11.14	+1945
$^{29}SiO_{4}$	92.95613	04.65	+1841
$^{186}W^{2}$	92.9754	28.41	+1332
$^{186}Os^{2}$	92.976/	01.59	+1321
$^{187}Re^{2}$	93.477/	62.93	-----
$^{187}Os^{2}$	93.478/	01.64	+94E3
$^{94}Ti_{2}$	93.90058	12.37	-13E3
$^{40}CaFe$	93.90247	05.64	-18E3
^{94}Mo	93.90594	09.04	-55E3
^{94}Zr	93.90764	17.40	-----
^{78}SeO	93.91230	23.47	+20E3
^{93}NbH	93.91348	99.985	+16E3
^{82}SeC	93.91663	09.09	+10E3
$^{62}NiO_{2}$	93.91814	03.64	+8944
$^{39}K_{2}O$	93.92233	86.47	+6393
$^{70}GeC_{2}$	93.92399	20.07	+5744
$^{94}FeC_{3}$	93.93331	00.39	+3658
$^{58}NiC_{3}$	93.93535	66.91	+3389
$^{46}TiO_{3}$	93.93736	07.94	+3160
$^{94}Si_{2}C_{3}$	93.95069	06.01	+2181
$^{46}TiC_{4}$	93.95263	07.65	+2087
$^{30}SiO_{4}$	93.95340	03.06	+2052
$^{31}P_{2}O_{2}$	93.95735	99.52	+1890
$^{188}Os^{2}$	93.9785/	13.3	+1325
$^{189}Os^{2}$	94.4793/	16.1	
$^{95}Ti_{2}$	94.89970	11.67	-20E3
$^{40}CaMn$	94.90091	96.97	-27E3
^{95}Mo	94.90444	15.72	-----
^{79}BrC	94.91330	50.42	+11E3
^{94}MoH	94.91376	09.04	+10E3
^{94}ZrH	94.91546	17.40	+8612
$^{40}CaFe$	95.89480	88.88	-6614
$^{96}Ti_{2}$	95.89589	56.38	-7152
^{96}Mo	95.90496	16.53	-22E3
^{96}Ru	95.9087	05.51	-16E4
^{96}Zr	95.90930	02.80	-----
^{80}SeO	95.91138	49.71	+46E3
^{95}MoH	95.91226	15.72	+32E3
^{84}SrC	95.91325	00.55	+24E3
$^{32}S_{3}$	95.91622	85.74	+14E3
$^{64}NiO_{2}$	95.91776	01.07	+11E3
$^{64}ZnO_{2}$	95.91896	48.65	+9928
$^{40}Ca_{2}O$	95.92008	93.22	+8897
$^{72}GeC_{2}$	95.92159	26.83	+7804
$^{60}NiC_{3}$	95.93077	25.40	+4467
$^{28}Si_{3}C$	95.93079	77.53	+4463
$^{48}TiO_{3}$	95.93265	73.45	+4107
$^{32}S_{2}O_{2}$	95.93396	89.82	+3889
$^{48}TiC_{4}$	95.94795	71.07	+2481
$^{32}SO_{4}$	95.95173	94.09	+2260
$^{192}Os^{2}$	95.9811/	41.0	+1336
$^{192}Pt^{2}$	95.9824/	00.78	+1312
$^{12}C_{8}$	96.00000	91.46	+1057
$^{193}Ir^{2}$	96.4834/	62.7	-----
$^{193}C^{2}_{16}$	96.50168	14.99	+5278
$^{97}Ti_{2}$	96.89581	08.93	-9318
$^{40}CaFe$	96.89827	02.12	-12E3
^{97}Mo	96.90621	09.46	-----
^{81}BrO	96.91133	49.34	+19E3
^{85}RbC	96.91202	71.35	+17E3
^{96}MoH	96.91278	16.53	+15E3
$^{97}S_{3}$	96.91561	02.06	+10E3
^{96}ZrH	96.91712	02.80	+8882
$^{65}CuO_{2}$	96.91758	30.76	+8523
$^{97}GeC_{2}$	96.92334	08.19	+5657
$^{97}Si_{3}C$	96.93035	12.73	+4014
$^{97}NiC_{3}$	96.93109	02.00	+3895
$^{49}TiO_{3}$	96.93257	05.47	+3676
$^{27}Al_{3}O$	96.93953	99.76	+2908
$^{97}TiC_{4}$	96.94787	08.44	+2326
$^{194}Pt^{2}$	96.9817/	32.9	+1284
$^{194}C^{2}_{16}$	97.00335	01.26	+ 998
$^{97}C_{8}$	97.00335	08.20	+ 998
$^{12}C_{8}H$	97.00782	91.45	+ 954
$^{195}Pt^{2}$	97.4831/	33.8	
$^{98}Ti_{2}$	97.89273	08.20	-7389
^{98}Mo	97.90598	23.78	-----
^{86}SrC	97.90935	09.75	+29E3
^{82}SeO	97.91154	09.18	+18E3
^{97}MoH	97.91403	09.46	+12E3
$^{98}S_{3}$	97.91201	11.43	+16E3
$^{85}Rb^{13}C$	97.91545	00.80	+10E3
$^{66}ZnO_{2}$	97.91585	27.68	+9920
$^{98}GeC_{2}$	97.92100	35.91	+6518
$^{74}SeC_{2}$	97.92254	00.85	+5912
$^{98}Si_{3}C$	97.92762	08.53	+4524
$^{98}NiC_{3}$	97.92834	03.58	+4379
$^{50}TiO_{3}$	97.92952	05.30	+4159
$^{50}CrO_{3}$	97.93078	04.28	+3948
$^{98}TiC_{4}$	97.94479	05.35	+2523
$^{50}CrC_{4}$	97.94605	04.12	+2443
$^{34}SO_{4}$	97.94752	04.18	+2357
^{98}Ru	97.954/	01.87	+2039
$^{31}P_{2}C_{3}$	97.96753	96.72	+1591
$^{196}Hg^{2}$	97.98291	00.146	+1273
$^{196}Pt^{2}$	97.9836	25.3	+1261
$^{98}C_{8}$	98.00670	00.321	+ 972
$^{12}C_{8}H_{2}$	98.01564	91.44	+ 893
$^{197}Au^{2}$	98.4836	100.00	
$^{99}Ti_{2}$	98.89266	00.59	-7387
^{99}Ru	98.90605	12.72	-----
^{99}SrC	98.90899	07.05	+34E3
^{87}RbC	98.90930	27.54	+30E3
^{98}MoH	98.91380	23.78	+13E3
$^{67}ZnO_{2}$	98.91694	04.09	+9082
$^{75}AsC_{2}$	98.92171	97.80	+6316
$^{63}CuC_{3}$	98.92959	66.82	+4202
$^{35}ClO_{4}$	98.94849	74.80	+2330
$^{198}Pt^{2}$	98.9823	07.21	+1297
$^{198}Hg^{2}$	98.98337	10.02	+1279
$C_{8}H_{3}$	99.02346	91.43	+ 842
$^{199}Hg^{2}$	99.48411	16.84	
$^{50}Ti_{2}$	99.88958	00.29	-5905
$^{50}Cr_{2}$	99.89210	00.19	-6933
^{100}Ru	99.905/	12.62	-67E3
^{100}SrC	99.90610	81.73	-25E4
^{100}Mo	99.90651	09.63	-----
^{84}SrO	99.90816	00.56	+60E3
$^{87}Rb^{13}C$	99.91265	27.54	+16E3
$^{68}ZnO_{2}$	99.91466	18.43	+12E3
$^{76}SeC_{2}$	99.91928	08.32	+7324
$^{76}GeC_{2}$	99.92129	07.59	+6760
$^{52}CrO_{3}$	99.92521	83.16	+5340
$^{29}Si_{3}O$	99.92570	78.21	+5203
$^{39}K_{2}C_{2}$	99.92742	84.77	+4778
$^{64}NiC_{3}$	99.92796	01.04	+4655
$^{64}ZnC_{3}$	99.92914	47.28	+4415
$^{52}CrC_{4}$	99.94051	80.11	+2938
$^{32}S_{2}C_{3}$	99.94414	87.29	+2654
$^{200}Hg^{2}$	99.98416	23.13	+1286
$C_{8}H_{4}$	100.03128	91.42	+ 801
$^{201}Hg^{2}$	100.48515	13.22	
^{101}Ru	100.905/	17.07	-----
^{89}YC	100.90572	98.89	+14E4
^{85}RbO	100.90693	71.93	+52E3
$^{88}Sr^{13}C$	100.90945	00.914	+23E3
^{100}MoH	100.91433	09.63	+11E3
$^{69}GaO_{2}$	100.91551	60.11	+9601
$^{101}SeC_{2}$	100.91998	07.61	+6736
$^{101}Si_{3}O$	100.92526	11.96	+4981
$^{53}CrO_{3}$	100.92538	09.48	+4951
$^{65}CuC_{3}$	100.92778	29.89	+4430
$^{101}CrC_{4}$	100.94065	12.72	+2830
$^{202}Hg^{2}$	100.98531	29.80	+1256
$C_{8}H_{5}$	101.03910	91.42	+ 752
$^{135}Ba^{32}$	101.17916	06.59	
$^{203}Tl^{2}$	101.4860	29.50	
$^{102}Cr_{2}$	101.88656	07.22	-5935
$^{51}V_{2}$	101.88795	99.52	-6458
^{102}Ru	101.90373	31.61	-----
^{86}SrO	101.90426	09.84	+19E4
^{90}ZrC	101.90433	50.89	+17E4
^{102}Pd	101.90486	00.96	+90E3
$^{89}Y^{13}C$	101.90907	01.107	+19E3
$^{70}GeO_{2}$	101.91379	20.42	+10E3
$^{102}SeC_{2}$	101.91739	23.15	+7460
$^{102}Si_{3}O$	101.92253	08.47	+5420
$^{54}CrO_{3}$	101.92360	02.36	+5129
$^{54}FeO_{3}$	101.92434	05.78	+4944
$^{66}ZnC_{3}$	101.92605	26.90	+4566
$^{136}Ba^{32}$	101.92828	07.81	+4151
$^{102}CrC_{4}$	101.93877	02.69	+2900
$^{54}FeC_{4}$	101.93961	05.57	+2840
$^{27}Al_{2}O_{3}$	101.94781	99.28	+2312
$^{204}Pb^{2}$	101.98654	01.48	+1231
$^{204}Hg^{2}$	101.98674	06.85	+1228
$^{12}C^{2}_{17}$	102.00000	82.72	+1059
$C_{8}H_{6}$	102.04692	91.41	+ 712
$^{205}Tl^{2}$	102.4869	70.50	-----
$^{205}C^{2}_{17}$	102.50168	15.75	+6934
$^{137}Ba^{32}$	102.67918	11.32	
$^{103}Cr_{2}$	102.88670	00.82	-5765
^{87}SrO	102.90390	07.00	-16E4
^{87}RbO	102.90421	27.78	-30E4
^{103}Rh	102.90455	100.00	-----
^{103}ZrC	102.90532	11.67	+13E4
$^{71}GaO_{2}$	102.91462	39.41	+10E3
$^{79}BrC_{2}$	102.91839	49.42	+7435
$^{55}MnO_{3}$	102.92278	99.28	+5645
$^{103}ZnC_{3}$	102.92714	04.88	+4555
$^{55}MnC_{4}$	102.93805	95.65	+3072
$^{39}KO_{4}$	102.94335	92.21	+2652
$^{206}Pb^{2}$	102.98722	23.6	+1245
$C_{8}H_{7}$	103.05474	91.40	+ 685
$^{207}Pb^{2}$	103.48794	22.6	-----
$^{138}Ba^{32}$	103.42866	71.66	1746
$^{104}Cr_{2}$	103.88102	70.37	-4668
^{88}SrO	103.90101	82.36	-46E3
^{104}Pd	103.90328	10.97	-----
^{104}Ru	103.90422	18.58	+11E4
^{104}ZrC	103.90467	17.04	+75E3
^{92}MoC	103.90855	15.66	+20E3
$^{72}GeO_{2}$	103.91139	27.30	+13E3
$^{80}SeC_{2}$	103.91647	48.72	+7877
$^{56}FeO_{3}$	103.91664	91.00	+7777
$^{104}ZnC_{3}$	103.92436	18.09	+4815
$^{40}Ca_{2}C_{2}$	103.92517	91.39	+4747
$^{56}FeC_{4}$	103.93194	87.67	+3625
$^{28}Si_{2}O_{3}$	103.93859	84.42	+2943
$^{40}CaO_{4}$	103.94250	96.04	+2649
$^{208}Pb^{2}$	103.98833	52.3	+1222
$C_{8}H_{8}$	104.06256	91.39	+ 652
$^{139}La^{32}$	104.17952	99.911	
$^{209}Bi^{2}$	104.48967	100.000	
$^{105}Cr_{2}$	104.88159	16.00	-4516
^{89}YO	104.90063	99.76	-25E3
^{105}Pd	104.90492	22.23	-----
^{93}NbC	104.90566	98.89	+13E4
$^{73}GeO_{2}$	104.91314	07.72	+13E3
$^{81}BrC_{2}$	104.91642	48.37	+9044
$^{57}FeO_{3}$	104.92011	02.17	+6861
$^{140}Ce^{32}$	104.92896	88.48	+4346
$^{105}FeC_{4}$	104.93541	06.02	+3429
$^{57}Si_{2}O_{3}$	104.93815	08.60	+3147
$^{27}Al_{3}C_{2}$	104.94462	97.80	+2636
$^{106}Cr_{2}$	105.87938	04.90	-4501
^{90}ZrO	105.89924	51.34	-29E3
^{106}Pd	105.90291	27.33	-----

$^{106}\mathrm{Pd}$	105.90291	27.33	-----
$^{106}\mathrm{Cd}$	105.90593	01.215	+35E3
$^{94}\mathrm{MoC}$	105.90594	08.94	+35E3
$^{94}\mathrm{ZrC}$	105.90764	17.21	+22E3
$^{93}\mathrm{Nb}^{13}\mathrm{C}$	105.90901	01.107	+17E3
$^{106}\mathrm{FeC_4}$	105.93331	00.41	+3484
$^{58}\mathrm{NiC_4}$	105.93525	66.17	+3265
$^{58}\mathrm{Si_2O_3}$	105.93542	05.88	+3258
$^{107}\mathrm{Cr_2}$	106.87592	00.46	-4224
$^{91}\mathrm{ZrO}$	106.90023	11.20	-23E3
$^{107}\mathrm{MoC}$	106.90444	10.68	-27E4
$^{107}\mathrm{Ag}$	106.90483	51.35	-----
$^{94}\mathrm{Zr}^{13}\mathrm{C}$	106.91099	00.193	+17E3
$^{75}\mathrm{AsO_2}$	106.91151	99.52	+16E3
$^{54}\mathrm{Cr_2}$	107.87774	00.06	-4194
$^{54}\mathrm{Fe_2}$	107.87922	00.34	-4450
$^{92}\mathrm{ZrO}$	107.89958	17.07	-28E3
$^{92}\mathrm{MoO}$	107.90346	15.80	-10E6
$^{108}\mathrm{Pd}$	107.90347	26.71	-----
$^{108}\mathrm{Cd}$	107.90407	00.875	+18E4
$^{108}\mathrm{MoC}$	107.90496	16.47	+72E3
$^{96}\mathrm{RuC}$	107.9087	05.45	+21E3
$^{76}\mathrm{SeO_2}$	107.90910	08.98	+19E3
$^{96}\mathrm{ZrC}$	107.90930	02.77	+19E3
$^{76}\mathrm{GeO_2}$	107.91111	07.72	+14E3
$^{84}\mathrm{SrC_2}$	107.91325	00.55	+11E3
$^{27}\mathrm{Al_4}$	107.92613	100.00	+4762
$^{60}\mathrm{NiC_4}$	107.93077	25.09	+3953
$^{28}\mathrm{Si_3C_2}$	107.93079	76.67	+3950
$^{44}\mathrm{CaO_4}$	107.93514	02.04	+3411
$^{12}\mathrm{C_9}$	108.00000	90.44	+1118
$^{217}\mathrm{C}_{18}^{2}$	108.50168	16.50	
$^{93}\mathrm{NbO}$	108.90057	99.76	-27E3
$^{109}\mathrm{Ag}$	108.90461	48.65	-----
$^{109}\mathrm{MoC}$	108.90621	09.54	+68E3
$^{77}\mathrm{SeO_2}$	108.90980	07.54	+21E3
$^{85}\mathrm{RbC_2}$	108.91202	70.56	+15E3
$^{96}\mathrm{Zr}^{13}\mathrm{C}$	108.91265	00.031	+14E3
$^{109}\mathrm{Si_3C_2}$	108.93035	13.50	+4231
$^{109}\mathrm{C_9}$	109.00336	09.12	+1103
$^{110}\mathrm{Fe_2}$	109.87155	10.67	-3463
$^{55}\mathrm{Mn_2}$	109.87611	100.00	-4044
$^{94}\mathrm{MoO}$	109.90085	09.02	-45E3
$^{94}\mathrm{ZrO}$	109.90255	17.36	-15E4
$^{110}\mathrm{Cd}$	109.90329	12.39	-----
$^{110}\mathrm{Pd}$	109.90447	11.81	+93E3
$^{110}\mathrm{MoC}$	109.90598	23.62	+41E3
$^{78}\mathrm{SeO_2}$	109.90721	23.42	+28E3
$^{86}\mathrm{SrC_2}$	109.90935	09.64	+18E3
$^{39}\mathrm{K_2O_2}$	109.91724	86.26	+7878
$^{110}\mathrm{Si_3C_2}$	109.92763	08.55	+4515
$^{46}\mathrm{TiO_4}$	109.93227	07.92	+3792
$^{31}\mathrm{P_2O_3}$	109.95226	99.28	+2244
$^{98}\mathrm{RuC}$	109.954/	01.85	+2167
$^{110}\mathrm{C_9}$	110.00670	00.409	+1063
$^{111}\mathrm{Fe_2}$	110.87502	00.26	-3790
$^{95}\mathrm{MoO}$	110.89935	10.73	-23E3
$^{111}\mathrm{Cd}$	110.90428	12.75	-----
$^{99}\mathrm{RuC}$	110.90605	12.58	+63E3
$^{79}\mathrm{BrO_2}$	110.90819	50.29	+28E3
$^{111}\mathrm{SrC_2}$	110.90899	07.09	+24E3
$^{87}\mathrm{RbC_2}$	110.90930	27.24	+22E3
$^{63}\mathrm{CuO_3}$	110.91432	68.59	+11E3
$^{63}\mathrm{CuC_4}$	110.92959	66.08	+4382
$^{47}\mathrm{TiO_4}$	110.93140	06.97	+4089
$^{111}\mathrm{C_9}$	111.01008	00.011	+1048
$^{112}\mathrm{Fe_2}$	111.86388	84.06	-2856
$^{112}\mathrm{Fe_2}$	111.87292	00.04	-3713
$^{96}\mathrm{MoO}$	111.89987	16.49	-35E3
$^{112}\mathrm{Cd}$	111.90306	24.07	-----
$^{96}\mathrm{RuO}$	111.90361	05.50	+20E4
$^{96}\mathrm{ZrO}$	111.90421	02.79	+97E3
$^{112}\mathrm{RuC}$	111.905	12.62	+58E3
$^{112}\mathrm{Sn}$	111.9051	00.96	+55E3
$^{112}\mathrm{SrC_2}$	111.9061	80.89	+37E3
$^{80}\mathrm{SeO_2}$	111.90629	49.36	+35E3
$^{100}\mathrm{MoC}$	111.90651	09.52	+32E3
$^{28}\mathrm{Si_4}$	111.90772	72.30	+24E3
$^{40}\mathrm{Ca_2O_2}$	111.91554	93.58	+8967
$^{48}\mathrm{TiO_4}$	111.92759	73.27	+4562
$^{64}\mathrm{ZnC_4}$	111.92796	46.76	+4494
$^{32}\mathrm{S_2O_3}$	111.92887	89.60	+4336
$^{113}\mathrm{Fe_2}$	112.86735	04.02	-3056
$^{97}\mathrm{MoO}$	112.90112	09.46	-36E3
$^{113}\mathrm{In}$	112.90430	04.28	-----
$^{113}\mathrm{Cd}$	112.90446	12.26	+71E4
$^{113}\mathrm{RuC}$	112.905	17.02	+16E4
$^{89}\mathrm{YC_2}$	112.90572	97.80	+80E3
$^{81}\mathrm{BrO_2}$	112.90622	49.22	+59E3
$^{65}\mathrm{CuO_3}$	112.91251	30.69	+14E3
$^{49}\mathrm{TiO_4}$	112.92751	05.46	+4867
$^{65}\mathrm{CuC_4}$	112.92778	29.56	+4809
$^{27}\mathrm{Al_3O_2}$	112.93444	99.52	+3746
$^{114}\mathrm{Fe_2}$	113.86525	00.66	-2974
$^{57}\mathrm{Fe_2}$	113.87082	00.05	-3481
$^{98}\mathrm{MoO}$	113.90089	23.72	-43E3
$^{114}\mathrm{Cd}$	113.90355	28.86	-----
$^{114}\mathrm{RuC}$	113.90373	31.45	+63E4
$^{114}\mathrm{Sn}$	113.9039	00.66	+33E4
$^{90}\mathrm{ZrC_2}$	113.90433	50.33	+15E4
$^{102}\mathrm{PdC}$	113.90486	00.95	+87E3
$^{82}\mathrm{SeO_2}$	113.90645	09.17	+39E3
$^{50}\mathrm{TiO_4}$	113.92443	05.29	+5455
$^{50}\mathrm{CrO_4}$	113.92569	04.27	+5145
$^{66}\mathrm{ZnC_4}$	113.92605	26.60	+5062
$^{98}\mathrm{RuO}$	113.949/	01.87	+2452
$^{12}\mathrm{C}_{18}^{2}$	114.00000	80.89	+1181
$^{99}\mathrm{RuO}$	114.90096	12.69	-43E3
$^{115}\mathrm{Sn}$	114.90335	00.35	-44E4
$^{115}\mathrm{In}$	114.90361	95.72	-----
$^{103}\mathrm{RhC}$	114.90455	98.89	+12E4
$^{115}\mathrm{ZrC_2}$	114.90532	12.10	+67E3
$^{90}\mathrm{Zr}^{25}\mathrm{C_2}$	114.90769	01.13	+28E3
$^{58}\mathrm{Ni_2}$	115.87070	47.86	-3681
$^{58}\mathrm{Fe_2}$	115.86662	00.001	-3258
$^{84}\mathrm{SrO_2}$	115.90305	00.56	-14E4
$^{100}\mathrm{RuO}$	115.900	12.59	-53E3
$^{100}\mathrm{MoO}$	115.90142	09.61	-15E4
$^{116}\mathrm{Sn}$	115.90219	14.30	-----
$^{104}\mathrm{PdC}$	115.90328	10.85	+11E4
$^{104}\mathrm{RuC}$	115.90422	18.37	+57E3
$^{116}\mathrm{ZrC_2}$	115.90467	16.98	+47E3
$^{116}\mathrm{Cd}$	115.90499	07.58	+41E3
$^{92}\mathrm{MoC_2}$	115.90855	15.49	+18E3
$^{52}\mathrm{CrO_4}$	115.92015	82.96	+6453
$^{28}\mathrm{Si_3O_2}$	115.92061	78.02	+6298
$^{116}\mathrm{ZnC_4}$	115.92486	17.94	+5113
$^{40}\mathrm{Ca_2C_3}$	115.92517	90.38	+5044
$^{232}\mathrm{Th}^{2}$	116.0190	100.00	+1185
$^{39}\mathrm{K_3}$	116.89113	80.70	-9766
$^{101}\mathrm{RuO}$	116.9000	17.03	-38E3
$^{85}\mathrm{RbO_2}$	116.90182	71.80	-91E3
$^{117}\mathrm{Sn}$	116.90310	07.61	-----
$^{117}\mathrm{PdC}$	116.90482	22.10	+68E3
$^{93}\mathrm{NbC_2}$	116.90566	97.80	+46E3
$^{85}\mathrm{Si_3O_2}$	116.92017	11.93	+6848
$^{53}\mathrm{CrO_4}$	116.92029	09.46	+6801
$^{27}\mathrm{Al_3C_2}$	116.94462	96.72	+2816
$^{234}\mathrm{U}^{2}$	117.0202	05.6E3	+ 998
$^{235}\mathrm{U}^{2}$	117.5214	00.72	
$^{118}\mathrm{Ni_2}$	117.86612	36.29	-3281
$^{59}\mathrm{Co_2}$	117.86636	100.00	-3304
$^{102}\mathrm{RuO}$	117.89864	31.53	-35E3
$^{86}\mathrm{SrO_2}$	117.89915	09.81	-41E3
$^{102}\mathrm{PdO}$	117.89977	00.96	-52E3
$^{118}\mathrm{Sn}$	117.90205	24.03	-----
$^{118}\mathrm{PdC}$	117.90291	27.28	+14E4
$^{106}\mathrm{CdC}$	117.90593	01.20	+30E3
$^{94}\mathrm{MoC_2}$	117.90594	08.84	+30E3
$^{94}\mathrm{ZrC_2}$	117.90764	17.02	+21E3
$^{86}\mathrm{Si_3O_2}$	117.91744	08.45	+7661
$^{54}\mathrm{CrO_4}$	117.91851	02.36	+7163
$^{54}\mathrm{FeO_4}$	117.91925	05.76	+6855
$^{119}\mathrm{Ni_2}$	118.86644	01.65	-3239
$^{119}\mathrm{K_3}$	118.88925	17.89	-8554
$^{87}\mathrm{SrO_2}$	118.89879	06.99	-27E3
$^{87}\mathrm{RbO_2}$	118.89912	27.72	-30E3
$^{103}\mathrm{RhO}$	118.89946	99.76	-32E3
$^{119}\mathrm{Sn}$	118.90315	08.58	-----
$^{119}\mathrm{MoC_2}$	118.90444	10.72	+92E3
$^{107}\mathrm{AgC}$	118.90483	50.78	+71E3
$^{55}\mathrm{MnO_4}$	118.91769	99.04	+8178
$^{238}\mathrm{U}^{2}$	119.0243	99.274	+ 981
$^{120}\mathrm{Ni_2}$	119.86154	11.94	-2949
$^{40}\mathrm{Ca_3}$	119.88776	90.34	-8303
$^{88}\mathrm{SrO_2}$	119.89592	82.16	-19E3
$^{104}\mathrm{PdO}$	119.89819	10.94	-30E3
$^{104}\mathrm{RuO}$	119.89914	18.53	-39E3
$^{120}\mathrm{Sn}$	119.90220	32.85	-----
$^{108}\mathrm{PdC}$	119.90347	26.41	+94E3
$^{108}\mathrm{CdC}$	119.90407	00.865	+64E3
$^{120}\mathrm{Te}$	119.90449	00.089	+52E3
$^{120}\mathrm{MoC_2}$	119.90496	16.41	+43E3
$^{96}\mathrm{RuC_2}$	119.9087	05.39	+18E3
$^{96}\mathrm{ZrC_2}$	119.90930	02.74	+17E3
$^{56}\mathrm{FeO_4}$	119.91158	90.78	+13E3
$^{27}\mathrm{Al_4C}$	119.92616	98.89	+5004
$^{28}\mathrm{Si_3C_3}$	119.93079	75.83	+4194
$^{12}\mathrm{C_{10}}$	120.00000	89.44	+1226
$^{121}\mathrm{Ni_2}$	120.86186	00.62	-2889
$^{121}\mathrm{K_3}$	120.88737	01.32	-7399
$^{89}\mathrm{YO_2}$	120.89552	99.52	-15E3
$^{105}\mathrm{PdO}$	120.89973	22.18	-30E3
$^{121}\mathrm{Sb}$	120.90371	57.25	-----
$^{109}\mathrm{AgC}$	120.90461	48.11	+13E4
$^{121}\mathrm{MoC_2}$	120.90621	09.61	+48E3
$^{57}\mathrm{FeO_4}$	120.91505	02.17	+11E3
$^{121}\mathrm{Si_3C_3}$	120.93035	14.14	+4538
$^{121}\mathrm{C_{10}}$	121.00335	10.02	+1213
$^{122}\mathrm{Ni_2}$	121.85911	03.41	-2784
$^{110}\mathrm{Fe_2C}$	121.87155	10.55	-3888
$^{55}\mathrm{Mn_2C}$	121.87610	98.89	-4549
$^{122}\mathrm{Ca_3}$	121.88435	01.79	-6572
$^{90}\mathrm{ZrO_2}$	121.89413	51.21	-14E3
$^{106}\mathrm{PdO}$	121.89782	27.26	-24E3
$^{106}\mathrm{CdO}$	121.90084	01.21	-59E3
$^{122}\mathrm{Te}$	121.90290	02.46	-----
$^{110}\mathrm{CdC}$	121.90329	12.25	+31E4
$^{110}\mathrm{PdC}$	121.90447	11.68	+78E3
$^{122}\mathrm{MoC_2}$	121.90598	23.47	+40E3
$^{86}\mathrm{SrC_3}$	121.90935	09.54	+19E3
$^{58}\mathrm{FeO_4}$	121.91295	00.33	+12E3
$^{58}\mathrm{NiO_4}$	121.91499	68.52	+10E3
$^{122}\mathrm{Si_3C_3}$	121.92762	08.60	+4931
$^{98}\mathrm{RuC_2}$	121.954/	01.83	+2386
$^{122}\mathrm{C_{10}}$	122.00670	00.505	+1174
$^{123}\mathrm{Ca_3}$	122.88678	00.41	-7063
$^{91}\mathrm{ZrO_2}$	122.89512	11.17	-14E3
$^{107}\mathrm{AgO}$	122.89974	51.23	-28E3
$^{123}\mathrm{Sb}$	122.90418	42.75	-----
$^{123}\mathrm{CdC}$	122.90428	12.75	+12E5
$^{123}\mathrm{Te}$	122.9043	00.87	+10E5
$^{123}\mathrm{RuC_2}$	122.90605	12.48	+66E3
$^{123}\mathrm{SrC_3}$	122.90899	07.11	+26E3
$^{87}\mathrm{RbC_3}$	122.90930	26.94	+24E3
$^{123}\mathrm{C_{10}}$	123.01008	00.015	+1161
$^{124}\mathrm{Ni_2}$	123.85873	00.57	-2664
$^{56}\mathrm{Fe_2C}$	123.86388	83.09	-3000
$^{124}\mathrm{Ca_3}$	123.88072	05.79	-5053
$^{92}\mathrm{ZrO_2}$	123.89447	17.03	-12E3
$^{92}\mathrm{MoO_2}$	123.89835	15.76	-18E3
$^{108}\mathrm{PdO}$	123.89838	26.55	-18E3
$^{108}\mathrm{CdO}$	123.89898	00.871	-20E3
$^{124}\mathrm{CdC}$	123.90306	23.94	-57E3
$^{124}\mathrm{Te}$	123.90312	04.61	-59E3
$^{124}\mathrm{RuC_2}$	123.905	12.62	-50E4
$^{124}\mathrm{Sn}$	123.90524	05.94	-----
$^{124}\mathrm{SrC_3}$	123.90610	80.08	+14E4
$^{124}\mathrm{Xe}$	123.90612	00.01	+14E4
$^{100}\mathrm{MoC_2}$	123.90651	09.42	+98E3
$^{60}\mathrm{NiO_4}$	123.91041	25.98	+24E3
$^{27}\mathrm{Al_4O}$	123.92107	99.76	+7827
$^{113}\mathrm{Fe_2C}$	124.86735	03.97	-3351
$^{93}\mathrm{NbO_2}$	124.89546	99.52	-14E3
$^{109}\mathrm{AgO}$	124.89952	48.53	-25E3
$^{113}\mathrm{InC}$	124.9043	04.23	-39E4
$^{125}\mathrm{CdC}$	124.90446	12.39	-78E4
$^{125}\mathrm{Te}$	124.90462	06.99	-----
$^{125}\mathrm{RuC_2}$	124.905	16.97	+33E4
$^{63}\mathrm{Cu_2}$	125.85918	47.73	-2817
$^{126}\mathrm{Fe_2C}$	125.86525	00.65	-3260
$^{94}\mathrm{MoO_2}$	125.89574	09.00	-16E3
$^{94}\mathrm{ZrO_2}$	125.89744	17.32	-20E3
$^{110}\mathrm{CdO}$	125.89820	12.36	-22E3
$^{110}\mathrm{PdO}$	125.89938	11.78	-28E3
$^{126}\mathrm{CdC}$	125.90355	28.68	-39E4
$^{126}\mathrm{RuC_2}$	125.90373	31.28	-90E4
$^{126}\mathrm{Te}$	125.90387	18.71	-----

^{126}Te	125.90387	18.71	-----
^{114}SnC	125.90320	00.65	+40E5
$^{90}ZrC_3$	125.90433	49.77	+27E4
^{126}Xe	125.90445	00.09	+22E4
$^{102}PdC_2$	125.90486	00.94	+13E4
$^{252}C^{2}_{21}$	126.00000	79.14	+1310
$^{95}MoO_2$	126.89424	10.71	-12E3
^{111}CdO	126.89919	12.72	-23E3
^{115}SnC	126.90335	00.35	-27E3
^{115}InC	126.90361	94.66	-12E4
$^{103}RhC_2$	126.90455	97.80	-72E5
^{127}I	126.90466	100.00	-----
$^{127}ZrC_3$	126.90532	12.52	+19E4
$^{63}CuO_4$	126.90923	68.43	+28E3
$^{254}C^{2}_{21}$	127.00335	02.085	+1286
$^{64}Zn_2$	127.85592	23.91	-2527
$^{128}Cu_2$	127.85737	42.71	-2655
$^{56}Fe_2O$	127.85879	83.81	-2735
$^{128}Ca_3$	127.88053	00.64	-5112
$^{52}Cr_2C_2$	127.88102	68.61	-5214
$^{96}MoO_2$	127.89476	16.45	-12E3
$^{96}RuO_2$	127.8985	05.48	-13E3
^{112}CdO	127.89797	23.95	-17E3
$^{96}ZrO_2$	127.89910	02.79	-20E3
^{112}SnO	127.9000	00.96	-23E3
^{116}SnC	127.90219	14.14	-38E3
$^{104}PdC_2$	127.90328	10.73	-56E3
^{128}Xe	127.90351	01.919	-63E3
$^{104}RuC_2$	127.90422	18.17	-96E3
$^{128}ZrC_3$	127.90467	16.91	-15E4
^{116}CdC	127.90499	07.50	-23E4
^{128}Te	127.90555	31.79	-----
$^{40}Ca_2O_3$	127.90990	92.78	+29E3
$^{97}MoO_2$	128.89601	09.41	-15E3
^{113}InO	128.89921	04.27	-23E3
^{113}CdO	128.89937	12.23	-24E3
^{129}SnC	128.9031	07.69	-79E3
^{129}Xe	128.90474	26.44	-----
$^{129}PdC_2$	128.90482	21.98	+16E5
$^{93}NbC_3$	128.90764	96.72	+45E3
$^{27}Al_3O_3$	128.92935	99.28	+5233
$^{130}Zn_2$	129.85401	27.20	-2452
$^{65}Cu_2$	129.85556	09.55	-2528
$^{98}MoO_2$	129.89578	23.67	-12E3
^{114}CdO	129.89846	28.79	-15E3
^{114}SnO	129.8983	00.66	-16E3
^{130}SnC	129.90205	23.92	-27E3
$^{130}PdC_2$	129.90291	27.22	-32E3
^{130}Xe	129.90350	04.08	-37E3
$^{106}CdC_2$	129.90593	01.19	-13E4
^{130}Ba	129.90623	00.101	-18E4
^{130}Te	129.90695	34.48	-----
$^{94}ZrC_3$	129.90764	16.83	+19E4
$^{131}Zn_2$	130.85510	04.02	-2619
$^{99}RuO_2$	130.89585	12.66	-14E3
^{115}SnO	130.89826	00.35	-19E3
^{115}InO	130.89852	95.40	-20E3
^{131}SnC	130.90315	08.78	-68E3
$^{107}AgC_2$	130.90485	50.22	-52E4
^{131}Xe	130.90508	21.18	-----
$^{132}Zn_2$	131.85282	25.89	-2522
$^{40}Ca_3C$	131.88776	89.34	-7598
$^{100}RuO_2$	131.8948	12.56	-13E3
$^{100}MoO_2$	131.89631	09.58	-15E3
^{116}SnO	131.89710	14.27	-16E3
^{116}CdO	131.89990	07.54	-25E3
^{132}SnC	131.90220	32.58	-45E3
$^{108}PdC_2$	131.90347	26.12	-80E3
$^{108}CdC_2$	131.90407	00.86	-13E4
^{132}Xe	131.90416	26.89	-14E4
^{120}TeC	131.90449	00.087	-21E4
^{132}Ba	131.90512	00.097	-----
$^{28}Si_3O_3$	131.91552	77.83	+13E3
$^{27}Al_4C_2$	131.92616	97.80	+6269
$^{12}C_{11}$	132.00000	88.45	+1390
$^{133}Zn_2$	132.85318	02.29	-2558
$^{101}RuO_2$	132.8948	16.99	-13E3
$^{85}RbO_3$	132.8968	71.63	-16E3
^{117}SnO	132.89801	07.59	-19E3
^{133}Cs	132.90513	100.00	-----
$^{109}AgC_2$	132.90461	47.58	+26E4
$^{85}RbC_4$	132.91202	69.01	+19E3
$^{85}Si_3O_3$	132.91508	11.90	+13E3
$^{133}C_{11}$	133.00335	10.90	+1353
$^{134}Zn_2$	133.85091	10.50	-2510
$^{67}Zn_2$	133.85428	00.17	-2680
$^{110}Fe_2C_2$	133.87155	10.43	-4094
$^{55}Mn_2C_2$	133.87610	97.80	-4757
$^{102}RuO_2$	133.89353	31.46	-13E3
$^{86}SrO_3$	133.89410	09.79	-13E3
^{118}SnO	133.89696	23.97	-18E3
^{122}TeC	133.9029	02.43	-99E3
$^{110}CdC_2$	133.90329	12.12	-14E4
^{122}SnC	133.90346	04.67	-17E4
^{134}Ba	133.90425	02.42	-----
$^{110}PdC_2$	133.90447	11.55	+61E4
$^{86}SrC_4$	133.90935	09.43	+26E3
$^{86}Si_3O_3$	133.91235	08.43	+17E3
$^{134}C_{11}$	134.00670	00.611	+1307
$^{135}Zn_2$	134.85200	01.53	-2519
$^{87}SrO_3$	134.89372	06.97	-11E3
$^{87}RbO_3$	134.89403	27.65	-12E3
$^{103}RhO_2$	134.89435	99.52	-12E3
^{119}SnO	134.89806	08.56	-18E3
^{123}SbC	134.90418	42.28	-98E3
$^{135}CdC_2$	134.90428	12.86	-11E4
^{135}Ba	134.90555	06.59	-----
$^{27}Al^{5}$	134.90770	100.00	+63E3
$^{68}Zn_2$	135.84972	03.45	-2487
$^{112}Fe_2C_2$	135.86388	82.20	-3356
$^{40}Ca_3O$	135.88267	90.12	-6263
$^{98}SrO_3$	135.89083	81.96	-10E3
$^{104}PdO_2$	135.89308	10.92	-12E3
$^{104}RuO_2$	135.89402	18.49	-13E3
^{120}SnO	135.89711	32.77	-19E3
^{120}TeO	135.89940	00.089	-27E3
^{124}TeC	135.89898	04.56	-25E3
$^{136}CdC_2$	135.90306	23.82	-10E4
^{136}Ba	135.90437	07.81	-----
$^{112}SnC_2$	135.9051	00.94	+19E4
^{124}SnC	135.90524	05.87	+16E4
$^{136}SrC_4$	135.90610	79.26	+79E3
^{136}Ce	135.90707	00.193	+50E3
^{136}Xe	135.90721	08.87	+48E3
$^{137}Fe_2C_2$	136.86735	05.77	-3582
$^{89}YO_3$	136.89042	99.28	-9037
$^{105}PdO_2$	136.89462	22.12	-13E3
^{121}SbO	136.89862	57.11	-20E3
$^{113}InC_2$	136.90430	04.19	-11E4
$^{137}CdC_2$	136.90446	12.52	-12E4
^{137}TeC	136.90462	06.96	-14E4
^{137}Ba	136.90557	11.32	-----
$^{69}Ga_2$	137.85142	36.48	-2580
$^{90}ZrO_3$	137.88906	51.09	-8717
$^{106}PdO_2$	137.89271	27.20	-12E3
$^{106}CdO_2$	137.89573	01.21	-15E3
^{122}TeO	137.89781	02.45	-20E3
^{122}SnO	137.89837	04.71	-21E3
$^{138}CdC_2$	137.90355	28.49	-10E4
^{138}TeC	137.90387	18.58	-14E4
$^{114}SnC_2$	137.9039	00.65	-14E4
$^{90}ZrC_4$	137.90433	49.22	-25E4
^{138}Ba	137.90488	71.66	-----
^{138}Ce	137.90603	00.25	+12E4
^{138}La	137.90674	00.089	+74E3
$^{91}ZrO_3$	138.89002	11.14	-8676
$^{107}AgO_2$	138.89463	51.10	-12E3
^{123}SbO	138.89909	42.65	-20E3
^{123}TeO	138.8992	00.87	-20E3
$^{139}SnC_2$	138.90335	00.35	-52E3
$^{115}InC_2$	138.90361	93.61	-57E3
^{127}IC	138.90466	98.89	-10E4
$^{139}ZrC_4$	138.90532	12.94	-20E4
^{139}La	138.90603	99.911	-----
^{139}BaH	138.91270	71.65	+20E3
$^{70}Ge_2$	139.84798	04.21	-2442
$^{140}Ga_2$	139.85053	47.84	-2555
$^{140}Ti_3$	139.85321	01.42	-2687
$^{28}Si_5$	139.88465	66.66	-6733
$^{92}ZrO_3$	139.88940	16.99	-8810
$^{108}PdO_2$	139.89327	26.58	-12E3
^{124}TeO	139.89803	04.58	-19E3
^{124}SnO	139.90015	05.93	-27E3
$^{116}SnC_2$	139.90219	13.99	-45E3
$^{140}ZrC_4$	139.90467	16.84	-23E4
$^{116}CdC_2$	139.90499	07.41	-48E4
^{140}Ce	139.90528	88.48	-----
^{128}TeC	139.90555	31.44	+52E4
^{139}LaH	139.91385	99.90	+16E3
$^{27}Al_4O_2$	[illegible]	[illegible]	+13E3
$^{141}Ti_3$	140.85234	02.63	-2555
$^{93}NbO_3$	140.89039	99.28	-8250
$^{109}AgO_2$	140.89441	48.42	-11E3
^{125}TeO	140.89953	06.96	-18E3
$^{141}SnC_2$	140.9031	07.75	-32E3
^{129}TeC	140.90555	31.44	-73E3
$^{93}NbC_4$	140.90566	95.65	-77E3
^{141}Pr	140.90743	100.00	-----
^{140}CeH	140.91310	88.47	+25E3
$^{142}Ge_2$	141.84558	11.23	-2227
$^{142}Ti_3$	141.84853	14.51	-2335
$^{71}Ga_2$	141.84964	15.68	-2379
$^{110}Fe_2O_2$	141.86137	10.62	-2961
$^{55}Mn_2O_2$	141.86592	99.52	-3271
$^{107}AgCl$	141.87368	38.78	-3984
$^{94}ZrO_3$	141.89237	17.27	-8382
$^{110}CdO_2$	141.89309	12.33	-8754
$^{110}PdO_2$	141.89427	11.75	-9442
^{126}TeO	141.89878	18.66	-14E3
$^{142}SnC_2$	141.90205	23.67	-20E3
^{130}BaC	141.90623	00.100	-46E3
^{130}TeC	141.90695	34.10	-60E3
^{142}Nd	141.90748	27.11	-78E3
$^{94}ZrC_4$	141.90764	16.64	-86E3
^{142}Ce	141.90930	11.07	-----
^{127}IO	142.89957	99.76	-14E3
$^{143}SnC_2$	142.90315	08.92	-22E3
^{143}Nd	142.90958	12.17	-----
^{142}NdH	142.91530	27.11	+25E3
^{142}CeH	142.91712	11.07	+19E3
$^{72}Ge_2$	143.84318	07.52	-2160
$^{144}Ti_3$	143.84385	44.17	-2182
$^{144}Ge_2$	143.84499	22.51	-2220
$^{56}Fe_2O_2$	143.85370	83.61	-2565
$^{109}AgCl$	143.87346	12.57	-3683
$^{40}Ca_3C_2$	143.88776	88.35	-6529
$^{112}CdO_2$	143.89286	23.95	-8495
^{128}TeO	143.90046	31.70	-15E3
$^{144}SnC_2$	143.9022	32.32	-19E3
^{132}BaC	143.90512	00.096	-31E3
^{144}Nd	143.90980	23.85	-----
^{144}Sm	143.91165	03.09	+78E3
$^{27}Al_4C_3$	143.92616	96.72	+8800
$^{12}C_{12}$	144.00000	37.46	+1595
$^{145}Ti_3$	144.84377	10.78	-2122
$^{145}Ge_2$	144.84493	04.15	-2159
$^{113}InO_2$	144.89410	04.26	-8069
$^{113}CdO_2$	144.89426	12.20	-8141
$^{121}SbC_2$	144.90371	55.99	-17E3
^{133}CsC	144.90513	98.89	-21E3
^{145}Nd	144.91206	08.30	-----
$^{145}C_{12}$	145.00335	11.76	+1587
$^{146}Ti_3$	145.84069	09.64	-2027
$^{146}Ge_2$	145.84259	23.83	-2081
$^{109}AgCl$	145.87051	11.90	-3459
$^{114}CdO_2$	145.89335	28.72	-7545
^{130}BaO	145.90114	00.101	-13E3
^{130}TeO	145.90186	34.30	-14E3
$^{122}TeC_2$	145.9029	02.41	-15E3
$^{122}SnC_2$	145.90346	04.62	-16E3
^{134}BaC	145.90425	02.39	-17E3
^{146}Nd	145.91269	17.22	-----
$^{146}C_{12}$	146.00670	00.725	+1552
$^{147}Ti_3$	146.84061	01.39	-1989
$^{147}Ge_2$	146.84434	05.67	-2094
$^{115}InO_2$	146.89341	95.26	-6969
$^{123}SbC_2$	146.90418	41.81	-14E3
^{147}BaC	146.90555	06.55	-16E3
$^{134}Ba^{13}C$	146.90760	00.026	-21E3
$^{27}Al_5C$	146.90770	98.39	-22E3
^{147}Sm	146.91449	14.97	-----
$^{147}C_{12}$	147.01003	00.027	+1537
$^{148}Ti_3$	147.83752	00.68	-1874
$^{148}Ge_2$	147.84200	17.61	-1987
$^{56}Fe_2O_3$	147.86388	81.26	-2313
$^{116}SnO_2$	147.89199	14.23	-6045
$^{116}CdO_2$	147.89479	07.54	-6826
$^{124}TeC_2$	147.89898	00.189	-8462
^{132}BaO	147.90003	00.097	-9000
^{148}BaC	147.90437	07.79	-12E3
$^{135}Ba^{13}C$	147.90891	00.07	-20E3
$^{124}SnC_2$	147.90524	05.81	-13E3
^{136}CeC	147.90707	00.191	-16E3
^{148}Sm	147.91442	11.24	-73E3
^{148}Nd	147.91646	05.73	-----

$^{149}Ge_2$	148.84463	01.20	-2063
$^{85}RbO_4$	148.89170	71.46	-5933
$^{117}SnO_2$	148.89290	07.57	-6230
^{133}CsO	148.90004	99.76	-8885
$^{149}TeC_2$	148.90462	06.94	-12E3
^{149}BaC	148.90557	11.28	-13E3
^{149}BaC	148.90772	00.086	-16E3
^{149}Sm	148.91680	13.83	-----
$^{150}Ge_2$	149.84229	05.67	-1909
$^{75}As_2$	149.84342	100.00	-1937
$^{86}SrO_4$	149.88899	09.77	-4712
^{134}BaO	149.89916	02.35	-6921
$^{150}TeC_2$	149.90387	18.45	-8845
^{150}BaC	149.90488	71.00	-9405
^{138}CeC	149.90603	00.25	-10E3
^{138}LaC	149.90674	00.088	-11E3
^{150}Sm	149.91690	07.44	-38E3
^{150}Nd	149.92082	05.62	-----
$^{87}SrO_4$	150.88863	06.95	-4883
$^{87}RbO_4$	150.88894	27.58	-4932
$^{119}SnO_2$	150.89295	08.54	-5676
^{135}BaO	150.90046	06.57	-7909
$^{27}Al_5O$	150.90261	99.76	-8914
$^{127}IC_2$	150.90466	97.80	-10E3
^{151}BaC	150.90824	00.79	-13E3
^{151}Eu	150.91954	47.82	-----
$^{152}Cr_3$	151.83261	00.47	-1751
$^{152}Se_2$	151.83856	01.22	-1880
$^{40}Ca_3O_2$	151.87758	89.91	-3636
$^{88}SrO_4$	151.88574	81.77	-4519
$^{120}SnO_2$	151.89200	32.69	-5553
^{136}BaO	151.89928	07.79	-7566
^{140}CeC	151.90528	87.50	-11E3
$^{128}TeC_2$	151.90555	31.09	-11E3
^{152}LaC	151.90938	01.106	-15E3
^{152}Sm	151.91936	26.72	-----
^{152}Gd	151.91943	00.20	+20E5
$^{153}Se_2$	152.83926	01.37	-1880
$^{89}YO_4$	152.88536	99.04	-4339
$^{121}SbO_2$	152.89351	56.97	-5645
^{137}BaO	152.90048	11.29	-7600
^{141}PrC	152.90748	98.89	-12E3
^{153}CeC	152.90863	00.979	-13E3
^{153}Eu	152.9206	52.18	-----
$^{154}Cr_3$	153.82707	09.07	-1623
$^{156}Se_2$	153.83667	05.68	-1805
$^{90}ZrO_4$	153.88397	50.97	-4055
$^{122}TeO_2$	153.8927	02.45	-5266
$^{122}SnO_2$	153.8933	04.70	-5376
^{138}BaO	153.89979	71.49	-6952
^{138}LaO	153.90165	00.089	-7590
^{138}CeO	153.90094	00.25	-7333
$^{130}BaC_2$	153.90623	00.099	-9804
$^{130}TeC_2$	153.90695	33.72	-10E3
^{142}NdC	153.90748	26.81	-11E3
^{142}CeC	153.9093	10.95	-12E3
^{154}Gd	153.92094	02.15	-16E4
^{154}Sm	153.92193	22.71	-----
$^{155}Cr_3$	154.82721	02.07	-1622
$^{155}Se_2$	154.83737	03.56	-1816
$^{91}ZrO_4$	154.88496	11.11	-4105
$^{123}SbO_2$	154.89398	42.54	-5394
^{139}LaO	154.90094	99.67	-7120
^{155}NdC	154.90958	12.30	-12E3
^{155}CeC	154.91265	00.123	-15E3
^{155}Gd	154.9227	14.73	-----
$^{156}Cr_3$	155.82153	59.40	-1548
$^{156}Se_2$	155.83575	14.68	-1802
$^{92}ZrO_4$	155.88431	16.95	-4108
$^{40}Ca_3C_3$	155.88776	87.37	-4519
$^{124}TeO_2$	155.88878	04.59	-4657
$^{124}SnO_2$	155.89504	05.91	-5728
$^{132}BaC_2$	155.90512	00.095	-9097
^{156}NdC	155.9098	23.72	-13E3
^{144}SmC	155.91165	03.06	-15E3
^{156}Gd	155.92226	20.47	-----
$^{156}C_{13}$	156.00000	86.49	+2006
$^{157}Cr_3$	156.82167	20.10	-1532
$^{157}Se_2$	156.83645	07.55	-1790
$^{93}NbO_4$	156.88530	99.04	-4044
$^{125}TeO_2$	156.89442	06.96	-5287
$^{133}CsC_2$	156.90513	97.80	-8272
^{141}PrO	156.90239	99.76	-7228
^{145}NdC	156.91206	08.47	-15E3
^{157}Gd	156.9241	15.68	-----
$^{157}C_{13}$	157.00335	12.60	+1980
$^{158}Cr_3$	157.81989	07.31	-1511
$^{158}Se_2$	157.83386	02.29	-1744
$^{79}Br_2$	157.83678	25.54	-1802
$^{94}ZrO_4$	157.88728	17.23	-4257
$^{126}TeO_2$	157.89367	18.62	-5139
^{142}NdO	157.90239	27.04	-7175
^{142}CeO	157.90421	11.04	-7822
$^{134}BaC_2$	157.90425	02.37	-7837
^{158}NdC	157.91269	17.12	-14E3
^{158}Dy	157.92401	00.09	-41E4
^{158}Gd	157.9244	24.87	-----
$^{158}C_{13}$	158.00335	00.847	+2000
$^{159}Cr_3$	158.82003	01.23	-1516
$^{159}Se_2$	158.83661	01.39	-1800
^{143}NdO	158.90449	12.14	-7794
$^{159}BaC_2$	158.90555	06.50	-8221
^{147}SmC	158.91449	14.80	-15E3
^{159}Tb	158.92488	100.00	-----
$^{159}C_{13}$	159.01008	00.038	+1865
$^{160}Se_2$	159.83294	29.14	-1696
$^{160}Br_2$	159.83481	49.99	-1731
$^{56}Fe_2O_3$	159.84861	83.41	-2035
$^{128}TeO_2$	159.8535	31.64	-2170
$^{160}BaC_2$	159.90437	07.78	-7000
^{144}NdO	159.90477	23.79	-7127
^{144}SmO	159.90656	03.08	-7745
$^{136}CeC_2$	159.90707	00.189	-7941
^{160}SmC	159.91442	11. 29	-13E3
^{148}NdC	159.91646	05.67	-15E3
^{160}Dy	159.9239	02.294	-48E3
^{160}Gd	159.92721	21.90	-----
$^{161}BaC_2$	160.90557	11.36	-7994
^{145}NdO	160.90697	08.28	-8592
^{161}SmC	160.9168	13.80	-18E3
^{161}Dy	160.9257	18.88	-----
$^{81}Br_2$	161.83284	24.47	-1746
$^{162}Se_2$	161.83310	09.15	-1751
$^{130}BaO_2$	161.89603	00.101	-5476
$^{130}TeO_2$	161.89675	34.31	-5613
$^{27}Al_6$	161.88924	100.00	-4453
$^{162}BaC_2$	161.90488	70.33	-7815
$^{138}CeC_2$	161.90603	00.245	-8274
^{162}SmC	161.9169	07.51	-19E3
^{150}NdC	161.92082	05.56	-34E3
^{162}Dy	161.9256	25.53	-----
^{162}Er	161.92873	00.136	+52E3
$^{163}BaC_2$	162.90824	01.57	-8330
$^{139}LaC_2$	162.90603	99.71	-7884
^{147}SmO	162.90940	14.93	-8855
^{151}EuC	162.91954	47.29	-20E3
^{163}Dy	162.9278	24.97	-----
$^{164}Fe_3$	163.81415	00.93	-1434
$^{164}Se_2$	163.83326	00.84	-1721
$^{132}BaO_2$	163.89492	00.097	-4882
$^{140}CeC_2$	163.90528	86.53	-7060
^{148}SmO	163.90933	11.21	-8551
^{148}NdO	163.91138	05.72	-9575
^{152}SmC	163.91936	26.42	-18E3
^{152}GdC	163.91943	00.198	-18E3
^{164}Dy	163.9285	28.18	-----
^{164}Er	163.9298	01.56	+13E3
$^{55}Mn_3$	164.81415	100.00	-1435
$^{133}CsO_2$	164.89493	99.52	-4827
$^{141}PrC_2$	164.90748	97.80	-7629
^{149}SmO	164.91171	13.80	-9484
^{153}EuC	164.9206	51.60	-19E3
$^{165}CeC_2$	164.90864	01.94	-8061
^{165}Ho	164.9291	100.00	-----
$^{166}Fe_3$	165.80349	14.67	-1325
$^{134}BaO_2$	165.89405	02.41	-4789
$^{142}NdC_2$	165.90748	26.51	-7819
$^{142}CeC_2$	165.90930	10.83	-8553
^{150}SmO	165.91181	07.42	-9824
^{150}NdO	165.91573	05.61	-13E3
^{154}GdC	165.92094	02.13	-21E3
^{154}SmC	165.92193	22.46	-44E3
^{166}Er	165.9287	33.41	-----
$^{167}Fe_2$	166.80995	00.70	-1385
$^{135}BaO_2$	166.89535	06.56	-4749
$^{167}NdC_2$	166.90958	12.49	-7979
$^{167}CeC_2$	166.91265	00.242	-9352
^{151}EuO	166.91445	47.70	-10E3
^{167}GdC	166.9227	14.59	-21E3
^{167}Er	166.9305	22.94	-----
$^{168}Fe_3$	167.79582	77.12	-1244
$^{28}Si_7$	167.86158	56.68	-2426
$^{40}Ca_3O_3$	167.87249	89.69	-2880
$^{136}BaO_2$	167.89417	07.77	-4585
$^{136}CeO_2$	167.89687	00.192	-4949
$^{168}NdC_2$	[illegible]	[illegible]	-7996
$^{144}SmC_2$	167.91165	03.02	-8769
^{156}DyC	167.914	00.052	-9996
^{152}SmO	167.91427	26.66	-10E3
^{152}GdO	167.91434	00.20	-10E3
^{168}GdC	167.92226	20.40	-21E3
^{168}Er	167.9308	27.07	-----
^{168}Yb	167.93390	00.135	+54E3
$^{12}C_{14}$	168.00000	85.53	+2427
$^{169}Fe_3$	168.79929	05.52	-1251
$^{137}BaO_2$	168,89537	11.27	-4335
$^{169}NdC_2$	168.91206	08.64	-7582
^{153}EuO	168.91551	52.05	-8972
^{169}GdC	168.9241	15.74	-17E3
^{169}Tm	168.93434	100.00	-----
$^{169}C_{14}$	169.00335	13.42	+2448
$^{170}Fe_3$	169.80319	00.96	-1283
$^{170}Sr_2$	169.82260	00.11	-1504
$^{85}Rb_2$	169.82404	52.06	-1523
$^{138}BaO_2$	169.89468	71.32	-4153
$^{138}CeO_2$	169.89585	00.25	-4275
$^{138}LaO_2$	169.89654	00.089	-4351
$^{134}BaC_3$	169.90425	02.34	-5421
$^{146}NdC_2$	169.91269	16.84	-7418
^{154}GdO	169.91585	02.14	-8604
^{154}SmO	169.91684	22.66	-9058
^{158}DyC	169.924	00.089	-15E3
^{170}GdC	169.9244	24.76	-15E3
^{170}Yb	169.934/	03.03	-11E4
^{170}Er	169.9356	14.88	-----
$^{170}C_{14}$	170.00670	00.977	+2390
$^{171}Sr_2$	170.82224	00.079	-1503
$^{139}LaO_2$	170.89583	97.43	-4255
$^{171}BaC_3$	170.90555	06.45	-5614
$^{147}SmC_2$	170.91449	14.64	-7947
^{155}GdO	170.91761	14.69	-9295
^{159}TbC	170.92488	98.89	-15E3
^{171}Yb	170.936/	14.31	-----
$^{171}C_{14}$	171.01008	00.044	+2307
$^{172}Sr_2$	171.81935	01.90	-1624
$^{172}Rb_2$	171.82132	40.19	-1655
$^{140}CeO_2$	171.89508	88.05	-5708
^{160}DyC	171.9239	02.27	-13E4
$^{172}BaC_3$	171.90437	07.76	-8254
^{156}DyO	171.909	00.052	-11E3
$^{172}SmC_2$	171.91442	11.31	-16E3
$^{148}NdC_2$	171.91646	05.60	-20E3
^{156}GdO	171.91717	20.42	-21E3
^{160}GdC	171.92721	21.66	-86E3
^{172}Yb	171.9252/	21.82	-----
$^{173}Sr_2$	172.81834	01.38	-1445
$^{141}PrO_2$	172.89728	99.52	-4247
$^{173}BaC_3$	172.90557	11.20	-5333
$^{173}SmC_2$	172.9168	13.78	-8157
^{157}GdO	172.91901	15.64	-9107
^{173}DyC	172.9257	18.70	-14E3
^{173}Yb	172.938/	16.13	-----
$^{58}Ni_3$	173.80605	33.11	-1455
$^{174}Sr_2$	173.81545	16.77	-1579
$^{174}Rb_2$	173.81860	07.76	-1625
$^{142}NdO_2$	173.89728	26.98	-6141
$^{142}CeO_2$	173.8991	11.02	-6563
$^{174}BaC_3$	173.90488	69.68	-8394
$^{174}SmC_2$	173.9169	07.58	-20E3
^{158}DyO	173.919	00.09	-26E3
^{158}GdO	173.91931	24.81	-28E3
$^{150}NdC_2$	173.92082	05.50	-36E3
^{174}DyC	173.9256	25.46	INF.
^{174}Yb	173.9256	31.84	-----
^{162}ErC	173.92873	00.134	+56E3
^{174}Hf	173.939	00.18	+13E3
$^{175}Sr_2$	174.81509	11.59	-1378
$^{143}NdO_2$	174.89938	12.11	-4105
$^{139}LaC_3$	174.90603	96.63	-4864
$^{151}EuC_2$	174.91954	46.77	-7789
^{159}TbO	174.91979	99.76	-7877
^{175}DyC	174.9278	24.97	-12E3
^{175}Lu	174.942/	97.41	-----
$^{176}Ni_3$	175.80147	37.66	-1246
$^{176}Sr_2$	175.81202	68.16	-1346
$^{144}NdO_2$	175.8996	23.74	-4080
$^{144}SmO_2$	175.90145	03.08	-4263
$^{140}CeC_3$	175.90528	85.57	-4699
^{160}DyO	175.91881	02.29	-7359
$^{152}SmC_2$	175.91936	26.13	-7532
$^{152}GdC_2$	175.91943	00.20	-7554
^{160}GdO	175.92212	21.85	-8541
^{176}DyC	175.9285	28.15	-12E3
^{164}ErC	175.9298	01.54	-14E3

^{176}Hf	175.92212	05.20	-8541
^{176}Lu	175.9419	02.59	-22E3
^{176}Yb	175.94272	12.73	-----
^{59}Co$_3$	176.79954	100.00	-1238
^{177}Ni$_3$	176.80179	01.71	-1257
^{145}NdO$_2$	176.90186	08.26	-4354
^{153}EuC$_2$	176.9206	51.03	-8080
^{161}DyO	176.92061	18.83	-8083
^{165}HoC	176.9291	98.89	-13E3
^{177}Hf	176.9425	18.50	-----
^{178}Ni$_3$	177.79689	19.53	-1218
^{89}Y$_2$	177.81144	100.00	-1353
^{146}NdO$_2$	177.90249	17.14	-4393
^{162}DyO	177.92051	25.47	-7912
^{154}GdC$_2$	177.92094	02.10	-8066
^{154}SmC$_2$	177.92193	22.21	-8445
^{162}ErO	177.92364	00.136	-9191
^{166}ErC	177.9287	33.04	-12E3
^{178}Hf	177.9430	27.14	-----
^{179}Ni$_3$	178.79720	01.30	-1209
^{147}SmO$_2$	178.90429	14.90	-4374
^{179}GdC$_2$	178.9227	14.73	-7953
^{163}DyO	178.92271	24.86	-7957
^{179}ErC	178.9305	23.05	-12E3
^{179}Hf	178.9452	13.75	-----
^{180}Ni$_3$	179.79446	07.37	-1187
^{90}Zr$_2$	179.80866	26.48	-1309
^{148}SmO$_2$	179.90422	26.48	-4297
^{148}NdO$_2$	179.9065	05.70	-4544
^{180}GdC$_2$	179.92226	20.34	-7548
^{164}DyO	179.92341	28.11	-7931
^{164}ErO	179.92471	01.56	-8413
^{180}ErC	179.9308	27.02	-12E3
^{168}YbC	179.9339	00.134	-15E3
^{180}W	179.9445	00.135	-11E4
^{180}Ta	179.945/	00.012	-16E4
^{180}Hf	179.9461	35.24	-----
^{12}C$_{15}$	180.00000	84.58	+3339
^{181}Ni$_3$	180.79262	00.43	-1181
^{181}Zr$_2$	180.80965	11.56	-1329
^{149}SmO$_2$	180.9066	13.76	-4616
^{165}HoO	180.9241	99.76	-8339
^{181}GdC$_2$	180.9241	15.78	-8339
^{169}TmC	180.9343	98.89	-16E3
^{181}Ta	180.9458	98.988	-----
^{181}C$_{15}$	181.00335	14.22	+3144
^{182}Ni$_3$	181.78987	02.22	-1165
^{182}Zr$_2$	181.80900	18.87	-1328
^{134}BaO$_3$	181.88898	02.40	-3191
^{134}BaC$_4$	181.90425	02.31	-4358
^{150}SmO$_2$	181.90670	07.40	-4630
^{150}NdO$_2$	181.91062	05.59	-5143
^{166}ErO	181.92361	33.33	-8126
^{182}GdC$_2$	181.924	24.66	-8270
^{170}YbC	181.934/	03.00	-15E3
^{170}ErC	181.9356	14.72	-18E3
^{182}W	181.9460	26.41	-----
^{182}C$_{15}$	182.00670	1.115	+2997
^{183}Zr$_2$	182.80999	03.84	-1325
^{183}Ni$_3$	182.79019	00.12	-1159
^{135}BaO$_3$	182.89028	06.54	-3164
^{183}BaC$_4$	182.90555	06.40	-4300
^{159}TbC$_2$	182.92488	97.80	-7879
^{167}ErO	182.92541	22.88	-8063
^{183}YbC	182.9360	14.18	-15E3
^{183}W	182.9481	14.40	-----
^{183}C$_{15}$	183.01008	00.054	+2952
^{184}Ni$_3$	183.78744	00.49	-1139
^{184}Zr$_2$	183.80934	20.83	-1318
^{184}Mo$_2$	183.81710	02.51	-1396
^{136}BaO$_3$	183.88910	07.75	-3076
^{184}BaC$_4$	183.90437	07.73	-4131
^{160}DyC$_2$	183.9239	02.24	-7358
^{152}SmO$_2$	183.90916	26.59	-4629
^{184}YbC	183.9252	21.74	-7762
^{168}ErO	183.9257	27.00	-7932
^{160}GdC$_2$	183.92721	21.41	-8481
^{168}YbO	183.9288	00.135	-9156
^{184}Os	183.946	00.018	-63E3
^{184}W	183.9489	30.64	-----
^{185}Ni$_3$	184.78776	00.03	-1154
^{185}Zr$_2$	184.81296	03.91	-1370
^{137}BaO$_3$	184.89030	11.24	-3205
^{153}EuO$_2$	184.9140	51.93	-4919
^{185}BaC$_4$	184.90557	11.17	-4359
^{185}DyC$_2$	184.9257	18.52	-8294
^{169}TmO	184.9292	99.76	-9843
^{185}YbC	184.938	16.37	-19E3
^{185}Re	184.948	37.07	-----
^{186}Ni$_3$	185.78501	00.09	-1122
^{93}Nb$_2$	185.81132	100.00	-1334
^{186}Zr$_2$	185.81231	08.83	-1344
^{186}Mo$_2$	185.81449	02.86	-1365
^{138}BaO$_3$	185.88961	71.14	-3044
^{186}BaC$_4$	185.90488	70.03	-4058
^{154}GdO$_2$	185.91074	02.14	-4653
^{154}SmO$_2$	185.91173	22.60	-4772
^{186}YbC	185.9256	31.67	-7408
^{186}DyC$_2$	185.9256	25.38	-7408
^{162}ErC$_2$	185.92873	00.133	-8464
^{170}YbO	185.9290	03.02	-8569
^{170}ErO	185.9356	14.84	-12E3
^{174}HfC	185.939	00.18	-16E3
^{186}W	185.9507	28.41	-----
^{186}Os	185.952	01.59	+14E4
^{187}Ni$_3$	186.78738	00.003	-1129
^{187}Mo$_2$	186.81299	04.98	-1335
^{187}Zr$_2$	186.81462	00.63	-1351
^{139}LaO$_3$	186.89076	99.19	-3004
^{155}GdO$_2$	186.9125	14.66	-4516
^{187}DyC$_2$	186.9278	24.98	-7419
^{171}YbO	186.9310	14.28	-8498
^{175}LuC	186.942	96.33	-17E3
^{187}Re	186.953/	62.93	-----
^{187}Os	186.956/	01.64	+62E3
^{188}Ni$_3$	187.78463	00.014	-1091
^{188}Zr$_2$	187.81528	03.99	-1327
^{188}Mo$_2$	187.81188	06.05	-1311
^{140}CeO$_3$	187.89001	87.84	-2810
^{140}CeC$_4$	187.90528	84.63	-3641
^{156}GdO$_2$	187.91206	20.37	-4192
^{172}YbO	187.9201	21.76	-5108
^{188}DyC$_2$	187.9285	28.11	-6618
^{164}ErC$_2$	187.9298	01.53	-6936
^{176}HfC	187.9408	05.14	-12E3
^{188}LuC	187.9419	03.64	-13E3
^{176}YbC	187.94272	12.59	-13E3
^{188}Os	187.9569	02.59	-----
^{63}Cu$_3$	188.78877	32.98	-1113
^{189}Mo$_2$	188.81476	05.84	-1315
^{27}Al$_7$	188.87078	100.00	-2154
^{157}GdO$_2$	188.91390	15.60	-4237
^{165}HoC$_2$	188.9291	97.80	-6427
^{173}YbO	188.9330	16.09	-7410
^{189}HfC	188.9425	18.36	-12E3
^{189}Os	188.9585	16.1	-----
^{190}Ni$_3$	189.78425	00.001	-1057
^{190}Mo$_2$	189.81453	12.99	-1271
^{190}Zr$_2$	189.81694	00.97	-1291
^{158}GdO$_2$	189.9142	24.75	-3815
^{174}YbO	189.9205	31.76	-4367
^{166}ErC$_2$	189.9287	32.67	-5381
^{174}HfO	189.9339	00.18	-6311
^{190}HfC	189.9430	27.04	-9046
^{190}Pt	189.964	00.013	-----
^{191}Cu$_3$	190.78696	44.26	-1082
^{191}Mo$_2$	190.80940	06.91	-1240
^{159}TbO$_2$	190.91468	99.52	-3920
^{191}ErC$_2$	190.9305	23.16	-5804
^{175}LuO	190.9369	97.18	-7206
^{191}HfC	190.9452	13.90	-11E3
^{191}Ir	190.9634	37.3	-----
^{64}Zn$_3$	191.78388	11.69	-1077
^{192}Mo$_2$	191.81192	13.05	-1277
^{96}Zr$_2$	191.81860	00.078	-1337
^{192}Ru$_2$	191.81740	00.31	-1326
^{160}DyO$_2$	191.9137	02.28	-3958
^{160}GdO$_2$	191.91703	21.80	-4250
^{192}ErC$_2$	191.9308	26.97	-6113
^{168}YbC$_2$	191.9339	00.132	-6783
^{176}HfO	191.9357	05.19	-7244
^{176}LuO	191.9368	02.58	-7558
^{176}YbO	191.9376	12.70	-7803
^{180}WC	191.9445	00.134	-11E3
^{180}TaC	191.945	00.012	-11E3
^{192}HfC	191.9461	35.00	-12E3
^{192}Os	191.9622	41.0	-----
^{192}Pt	191.9648	00.78	+74E3
^{12}C$_{16}$	192.00000	83.64	+5078
^{193}Cu$_3$	192.78515	19.80	-1063
^{193}Mo$_2$	192.81042	10.60	-1235
^{161}DyO$_2$	192.9155	18.79	-3769
^{169}TmC$_2$	192.9343	97.80	-5956
^{177}HfO	192.9374	18.46	-6586
^{181}TaC	192.9458	98.88	-9233
^{193}Ir	192.9667/	62.7	-----
^{193}C$_{16}$	193.00335	14.99	+5265
^{194}Zn$_3$	193.78197	19.95	-1070
^{194}Mo$_2$	193.81094	10.49	-1273
^{194}Ru$_2$	193.86270	00.21	-1928
^{162}DyO$_2$	193.9154	25.41	-4049
^{170}YbC$_2$	193.934	02.96	-6620
^{170}ErC$_2$	193.9356	14.55	-7002
^{178}HfO	193.9379	27.07	-7636
^{182}WC	193.9460	26.12	-11E3
^{194}Pt	193.9633/	32.9	-----
^{194}C$_{16}$	194.00670	01.26	+4469
^{195}Zn$_3$	194.78306	02.95	-1065
^{195}Mo$_2$	194.81219	07.53	-1266
^{195}Ru$_2$	194.81475	01.40	-1237
^{163}DyO$_2$	194.91760	24.85	-4012
^{195}YbC$_2$	194.9360	14.06	-6456
^{179}HfO	194.9401	13.72	-7470
^{195}WC	194.9481	14.53	-11E3
^{195}Pt	194.9662/	33.8	-----
^{195}C$_{16}$	195.01008	00.066	+4443
^{196}Zn$_3$	195.78078	24.65	-1052
^{196}Mo$_2$	195.81196	08.84	-1263
^{196}Ru$_2$	195.81370	01.43	-1277
^{28}Si$_7$	195.83851	56.68	-1524
^{164}ErO$_2$	195.91960	01.55	-4126
^{164}DyO$_2$	195.92340	28.04	-4484
^{196}YbC$_2$	195.9252	21.65	-4677
^{180}WO	195.9394	00.135	-7075
^{180}HfO	195.9410	35.16	-7508
^{180}TaO	195.9399	00.012	-7205
^{184}OsC	195.946/	00.018	-9288
^{196}WC	195.9489	30.46	-11E3
^{196}Hg	195.96583	00.146	-15E4
^{196}Pt	195.9671/	25.3	-----
^{197}Zn$_3$	196.78115	03.35	-1059
^{197}Mo$_2$	196.81272	01.82	-1275
^{197}Ru$_2$	196.81370	02.36	-1283
^{197}Si$_7$	196.83806	20.22	-1525
^{165}HoO$_2$	196.9189	99.52	-4078
^{197}YbC$_2$	196.938/	16.24	-6745
^{181}TaO	196.9407	99.747	-7432
^{185}ReC	196.948/	36.66	-10E3
^{197}Au	196.9672	100.00	-----
^{198}Zn$_3$	197.77814	17.99	-1062
^{198}Ru$_2$	197.81243	05.57	-1298
^{198}Mo$_2$	197.81249	04.58	-1301
^{198}Si$_7$	197.83533	16.39	-1531
^{134}BaO$_4$	197.88390	02.40	-2453
^{166}ErO$_2$	197.9185	33.25	-4294
^{198}YbC$_2$	197.9256	31.14	-5076
^{174}HfC$_2$	197.939/	00.75	-7733
^{182}WO	197.9409	26.65	-8353
^{186}WC	197.9507	28.10	-14E3
^{186}OsC	197.952/	01.57	-16E3
^{198}Pt	197.9646	07.21	-----
^{198}Hg	197.96675	10.02	+92E3
^{199}Zn$_3$	198.77996	03.19	-1057
^{199}Ru$_2$	198.8111	03.84	-1266
^{199}Si$_7$	198.83489	04.33	-1492
^{135}BaO$_4$	198.88519	06.53	-2397
^{167}ErO$_2$	198.9203	22.83	-4152
^{175}LuC$_2$	198.942/	95.27	-7588
^{183}WO	198.9430	14.33	-7889
^{187}ReC	198.953/	62.23	-13E3
^{187}OsC	198.956/	01.62	-16E3
^{199}Hg	198.96822	16.84	-----
^{200}Zn$_3$	199.77696	10.01	-1045
^{200}Ru$_2$	199.81110	09.16	-1263
^{200}Mo$_2$	199.81302	00.93	-1288
^{200}Si$_7$	199.83216	01.37	-1469
^{136}BaO$_4$	199.88401	07.73	-2371
^{168}ErO$_2$	199.92060	26.94	-4190
^{178}HfC$_2$	199.9408	05.09	-7264
^{200}LuC$_2$	199.9419	04.66	-7317
^{176}YbC$_2$	199.94272	12.45	-7308
^{184}OsO	199.9409	00.018	-7290
^{184}WO	199.9438	30.57	-8152
^{188}OsC	199.9569	13.2	-13E3
^{200}Hg	199.96833	22.13	-----

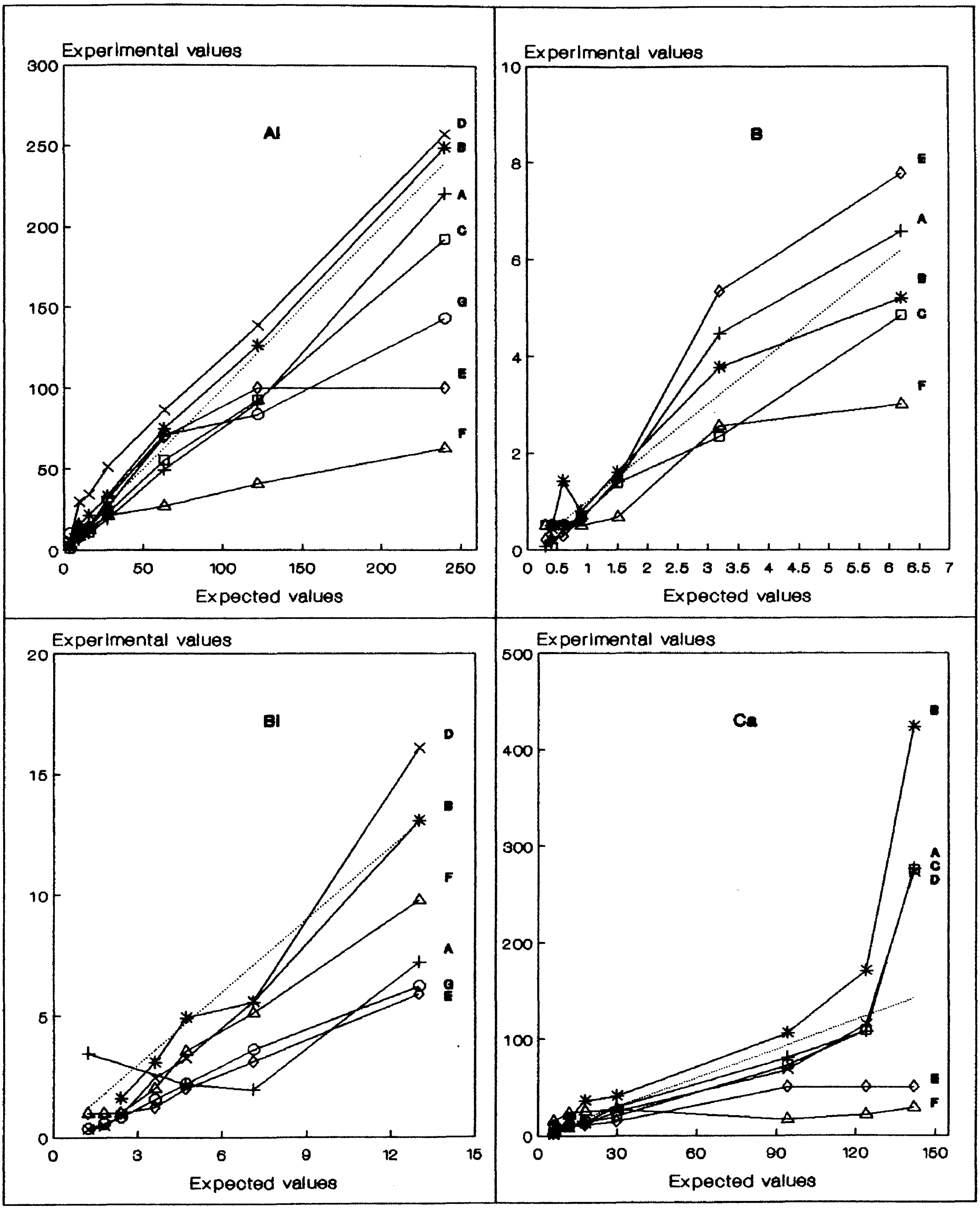
$^{201}Zn_3$	200.77805	01.36	-1045
$^{201}Ru_2$	200.80978	12.35	-1252
$^{137}BaO_4$	200.88521	11.21	-2362
$^{169}TmO_2$	200.9241	99.52	-4351
$^{201}HfC_2$	200.9425	18.20	-7232
^{185}ReO	200.943/	36.98	-7364
^{201}OsC	200.9585	16.0	-17E3
^{201}Hg	200.97209	13.22	-----
$^{202}Zn_3$	201.77577	03.45	-1037
$^{202}Ru_2$	201.8087	11.58	-1247
$^{138}BaO_4$	201.88452	70.97	-2346
$^{170}YbO_2$	201.9238	03.03	-4313
$^{170}ErO_2$	201.9254	14.81	-4467
$^{202}HfC_2$	201.9430	26.95	-7311
^{186}WO	201.9456	28.35	-8071
^{202}OsC	201.9548	26.3	-13E3
^{202}Hg	201.97063	29.80	-----
$^{203}Zn_3$	202.77685	00.47	-1041
$^{203}Ru_2$	202.8087/	15.52	-1244
$^{171}YbO_2$	202.9258	14.24	-4403
$^{203}HfC_2$	202.9452	14.04	-7602
^{187}ReO	202.948/	62.78	-8493
^{187}OsO	202.9510	01.64	-9712
^{191}IrC	202.9634	37.3	-24E3
^{203}Tl	202.9719	29.50	-----
$^{204}Zn_3$	203.77451	00.84	-1027
$^{204}Ru_2$	203.80746	14.68	-1232
$^{140}CeO_4$	203.88492	87.63	-2314
$^{172}YbO_2$	203.9150	21.71	-3512
$^{180}WC_2$	203.9445	00.132	-7137
$^{180}TaC_2$	203.9458	00.012	-7477
$^{204}HfC_2$	203.9461	34.76	-7560
^{192}OsC	203.9622	40.55	-19E3
^{192}PtC	203.9648	00.77	-25E3
^{204}Pb	203.97308	01.48	-----
^{204}Hg	203.97347	06.85	+52E4
$^{12}C_{17}$	204.00000	82.72	+7577
$^{205}Zn_3$	204.77505	00.067	-1031
$^{205}Ru_2$	204.8092	06.34	-1245
$^{173}YbO_2$	204.9278	16.05	-4456
$^{181}TaC_2$	204.9458	97.79	-7320
^{189}OsO	204.9534	16.1	-10E3
^{193}IrC	204.9667	62.0	-29E3
^{205}Tl	204.9738	70.50	-----
$^{205}C_{17}$	205.00335	15.75	+6937
$^{206}Zn_3$	205.77505	00.067	-1033
$^{206}Ru_2$	205.80795	11.75	-1237
$^{206}Pd_2$	205.80814	00.21	-1239
$^{206}Rh_2$	205.80910	100.00	-1246
$^{174}YbO_2$	205.9154	31.69	-3489
$^{182}WC_2$	205.9460	25.83	-7242
^{190}OsO	205.9497	26.3	-8326
^{194}PtC	205.9633	32.5	-18E3
^{206}Pb	205.97444	26.4	-----
$^{206}C_{17}$	206.00670	01.41	+6385
$^{207}Pd_2$	206.80968	00.43	-1245
$^{175}LuO_2$	206.9318	96.94	-4695
$^{207}WC_2$	206.9481	14.66	-7451
^{191}IrO	206.9583	37.2	-12E3
^{207}PtC	206.9662	33.8	-21E3
^{207}Pb	206.97588	22.6	-----
$^{207}C_{17}$	207.01008	00.079	+6052
$^{208}Zn_3$	207.77554	00.002	-1034
$^{208}Pd_2$	207.80656	01.73	-1223
$^{208}Ru_2$	207.80844	03.45	-1236
$^{176}HfO_2$	207.9306	05.17	-4516
$^{176}LuO_2$	207.9317	02.58	-4627
$^{176}YbO_2$	207.9325	12.67	-4711
$^{208}WC_2$	207.9489	30.29	-7495
^{192}OsO	207.9571	40.9	-11E3
^{192}PtO	207.9579	00.78	-13E3
^{208}PtC	207.9671	25.37	-22E3
^{208}Pb	207.97665	52.3	-----
$^{209}Pd_2$	208.80810	04.88	-1220
$^{177}HfO_2$	208.9323	18.41	-4443
$^{185}ReC_2$	208.948	36.25	-6668
^{193}IrO	208.9616	62.5	-12E3
^{197}AuC	208.9672	98.89	-17E3
^{209}Bi	208.97934	100.00	-----
$^{210}Pd_2$	209.80619	11.45	-1381
$^{178}HfO_2$	209.80964	27.01	-8266
$^{186}WC_2$	209.9507	27.78	-28E3
$^{188}OsC_2$	209.952	01.55	-34E3
^{194}PtO	209.9582	32.8	-----
^{198}PtC	209.9646	07.13	+33E3
^{211}HgC	209.96675	16.76	+25E3
$^{211}Pd_2$	210.80773	12.15	-1376
$^{187}ReC_2$	210.953	61.54	-27E3
^{195}PtO	210.9611	33.7	-----
^{199}HgC	210.96822	16.65	+30E3
$^{212}Pd_2$	211.80582	13.55	-1357
$^{180}HfO_2$	211.9359	35.07	-8121
^{196}PtO	211.9620	25.2	-----
^{212}HgC	211.96833	23.06	+34E3
$^{213}Pd_2$	212.80829	11.88	-1385
$^{181}TaO_2$	212.9356	99.51	-8036
^{197}AuO	212.9621	99.76	-----
^{213}HgC	212.97029	13.33	+26E3
$^{214}Pd_2$	213.80638	17.19	-1378
$^{214}Ag_2$	213.80966	26.37	-1408
$^{187}WO_2$	213.9358	26.28	-8274
^{198}PtO	213.9595	02.19	-99E3
^{198}HgO	213.96166	10.00	-----
^{214}HgC	213.97063	29.62	+24E3
$^{215}Pd_2$	214.80695	05.25	-1397
$^{183}WO_2$	214.9379	14.33	-8520
^{199}HgO	214.96313	16.80	-----
^{203}TlC	214.9719	29.17	+25E3
$^{216}Pd_2$	215.80694	13.58	-1119
$^{216}Ag_2$	215.80944	49.96	-1134
$^{184}WO_2$	215.9387	30.49	-3524
^{200}HgO	215.96323	23.07	-5874
^{204}PbC	215.97308	01.46	-8024
^{204}HgC	215.97347	06.77	-8142
$^{12}C_{18}$	216.00000	81.80	-----
$^{217}Cd_2$	216.81021	00.31	-1124
$^{186}WO_2$	216.9405	28.27	-5688
^{205}TlC	216.9738	69.72	-7344
$^{217}C_{18}$	217.00335	16.50	-----
$^{218}Cd_2$	217.80736	00.80	-1094
$^{218}Pd_2$	217.80794	06.31	-1097
$^{218}Ag_2$	217.80922	23.67	-1104
^{202}HgO	217.96553	29.73	-5295
^{206}PbC	217.97444	23.3	-6758
$^{218}C_{18}$	218.00670	01.571	-----
$^{219}Cd_2$	218.80835	00.52	-1086
^{203}TlO	218.9668	29.43	-5060
^{219}PbC	218.97588	22.7	-6404
$^{219}C_{18}$	219.01008	00.094	-----
$^{220}Cd_2$	219.80658	02.66	-1363
$^{220}Pd_2$	219.80894	01.39	-1383
^{204}PbO	219.96799	01.48	-----
^{204}HgO	219.96838	06.83	+57E4
^{220}PbC	219.97665	52.0	+25E3
$^{221}Cd_2$	220.80757	03.37	-1371
^{205}TlO	220.9687	70.3	-----
^{209}BiC	220.97934	98.89	+21E3
$^{222}Cd_2$	221.80635	08.28	-1362
^{206}PbO	221.96935	23.5	-----
$^{223}Cd_2$	222.80734	08.27	-1364
^{207}PbO	222.97080	22.5	-----
$^{224}Cd_2$	223.80684	16.20	-1360
$^{224}Si_8$	223.81544	52.27	-1435
^{208}PbO	223.97156	52.1	-----
$^{75}As_3$	224.76513	100.00	-1076
$^{225}Cd_2$	224.80783	13.26	-1352
^{209}BiO	224.97425	99.76	-----
$^{226}Cd_2$	225.80661	17.27	
$^{227}Cd_2$	226.80801	09.01	
$^{228}Cd_2$	227.80710	11.98	-1182
$^{228}In_2$	227.80791	08.19	-1188
$^{204}PbC_2$	227.97308	01.45	-8470
$^{228}C_{19}$	228.00000	80.89	-----
$^{229}Cd_2$	228.80945	01.86	-1181
$^{229}C_{19}$	229.00335	17.22	-----
$^{230}In_2$	229.80722	91.62	-1153
$^{230}Cd_2$	229.80854	04.38	-1161
$^{230}C_{19}$	230.00670	01.74	-----
$^{231}PbC_2$	230.97588	22.6	
$^{232}Sn_2$	231.80638	03.05	-1002
$^{232}Cd_2$	231.80998	00.57	-1018
$^{232}PbC_2$	231.97665	51.6	-3782
^{232}Th	232.0380	100.00	-----
$^{233}Sn_2$	232.80529	02.46	-----
$^{209}BiC_2$	232.97934	97.80	+1338
$^{234}Sn_2$	233.80424	08.04	- 991
^{234}U	234.0403	00.0056	----
$^{235}Sn_2$	234.80515	06.34	- 989
^{235}U	235.0428	00.7204	----
$^{236}Sn_2$	235.80439	16.65	
$^{237}Sn_2$	236.80530	09.16	-1497
$^{205}TlO_2$	236.9636	70.20	-----
$^{238}Sn_2$	237.80425	17.95	- 974
$^{206}PbO_2$	237.96424	23.5	-2822
^{238}U	238.0486	99.2739	----
$^{239}Sn_2$	238.80535	06.40	-1490
$^{207}PbO_2$	238.96568	22.5	-----
$^{240}Sn_2$	239.80440	14.76	-1227
$^{208}PbO_2$	239.96645	52.0	-7154
$^{240}C_{20}$	240.00000	79.99	-----
$^{241}Sn_2$	240.80661	01.71	-1225
$^{241}C_{20}$	241.00335	17.93	-----
$^{242}Sn_2$	241.80566	05.96	-1204
$^{242}C_{20}$	242.00670	01.91	-----
$^{243}Sn_2$	242.80839	01.02	-1205
$^{243}C_{20}$	243.01008	00.128	-----
$^{244}Sn_2$	243.80692	04.13	
^{232}ThC	244.0380	98.89	
^{232}ThO	248.0329	99.76	
^{238}UC	250.0486	98.175	
$^{252}C_{21}$	252.00000	79.14	
$^{253}C_{21}$	253.00335	18.62	
$^{254}C_{21}$	254.00670	02.09	-----
^{238}UO	254.0435	99.035	+5930
$^{232}ThC_2$	256.0380	97.80	
$^{238}UC_2$	262.0486	97.088	
$^{232}ThO_2$	264.0278	99.52	9496
$^{264}C_{22}$	264.00000	78.26	-----
$^{265}C_{22}$	265.00335	19.29	
$^{266}C_{22}$	266.00670	02.27	
$^{238}UO_2$	270.0384	98.796	

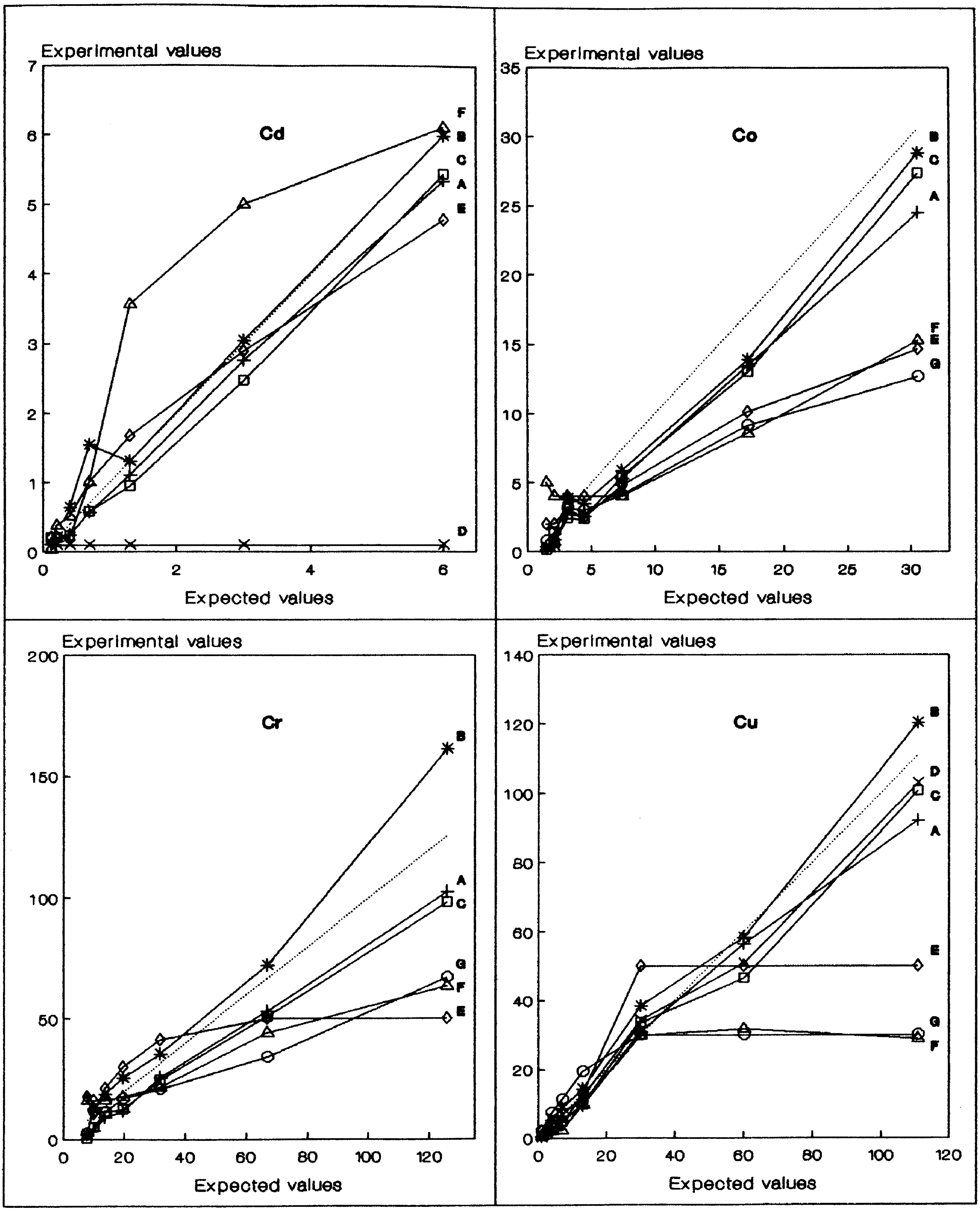
APPENDIX C

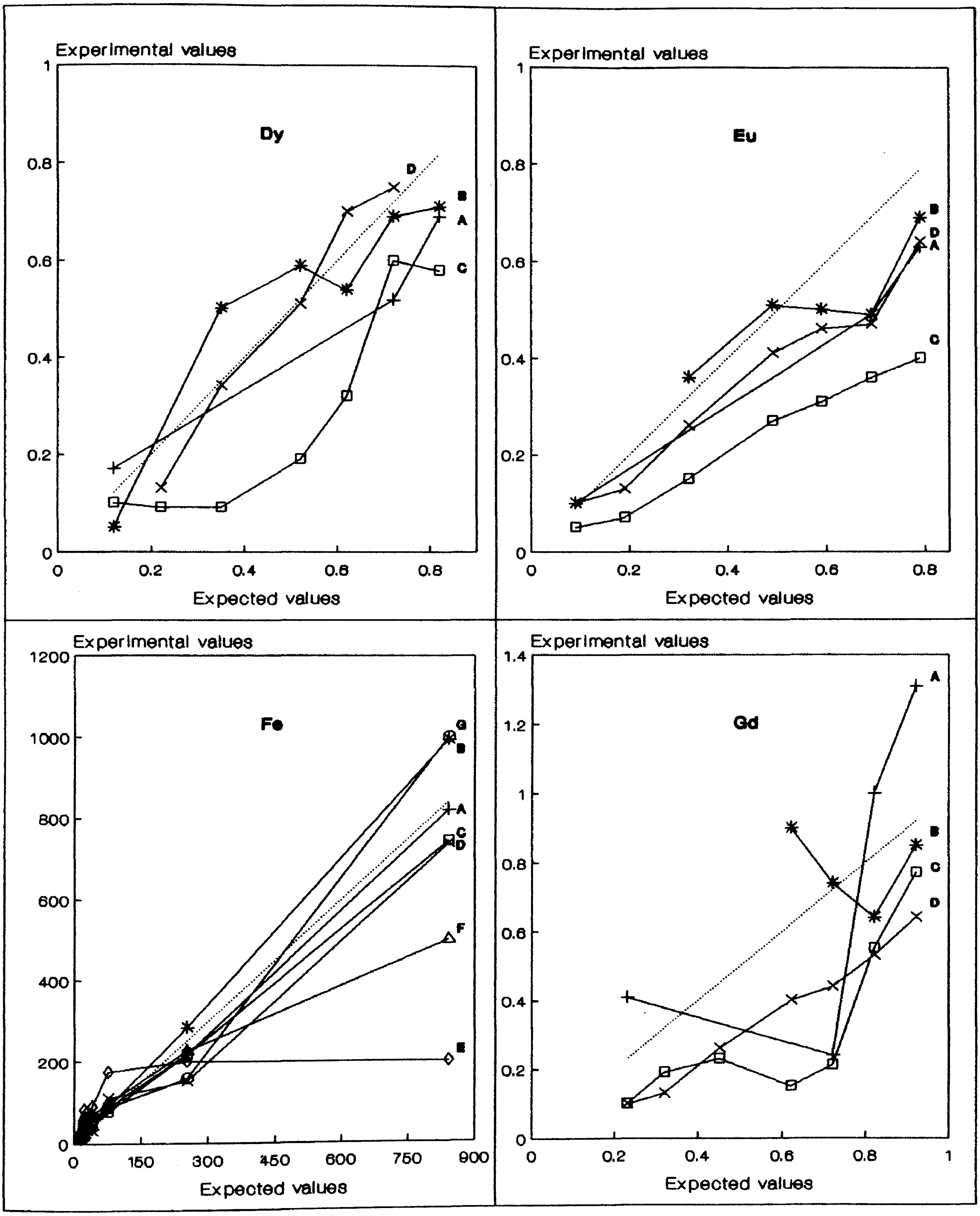
COMPARISON OF EXPERIMENTAL ANALYTICAL DATA TO EXPECTED VALUES FOR SELECTED ELEMENTS USING VARIOUS ANALYTICAL TECHNIQUES

Laboratory	*Analytical Method*
A	*Inductively coupled plasma (ICP) optical emission spectroscopy (OES)*
B	*Spark-source mass spectrometry (SSMS)*
C	*Inductively coupled plasma (ICP) optical emission spectroscopy (OES)*
D	*Atomic absorption spectroscopy (AAS)*
E	*Arc emission spectroscopy (AES) (AgCl buffer)*
F	*Arc emission spectroscopy (AES) (NaCl buffer)*
G	*Direct current emission spectroscopy*

Experimental and expected values are given in the units μgX/gU. The dotted lines depict expected concentrations.


Experimental values
300
250
200
150
100
50
0
Al
D
B
A
C
G
E
F
0
50
100
150
200
250
Expected values
Experimental values
10
8
6
4
2
0
B
E
A
B
C
F
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
Expected values
Experimental values
20
15
10
5
0
Bi
D
B
F
A
G
E
0
3
6
9
12
15
Expected values
Experimental values
500
400
300
200
100
0
Ca
B
A
C
D
E
F
0
30
60
90
120
150
Expected values


Experimental values
7
6
5
4
3
2
1
0
Cd
F
B
C
A
E
D
0
2
4
6
Expected values
Experimental values
35
30
25
20
15
10
5
0
Co
B
C
A
F
E
G
0
5
10
15
20
25
30
Expected values
Experimental values
200
150
100
50
0
Cr
B
A
C
G
F
E
0
20
40
60
80
100
120
Expected values
Experimental values
140
120
100
80
60
40
20
0
Cu
B
D
C
A
E
G
F
0
20
40
60
80
100
120
Expected values


Experimental values
Dy
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
Expected values
D
B
A
C
Experimental values
Eu
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
Expected values
B
D
A
C
Experimental values
Fe
1200
1000
800
600
400
200
0
0
150
300
450
600
750
900
Expected values
G
B
A
C
D
F
E
Experimental values
Gd
1.4
1.2
1
0.8
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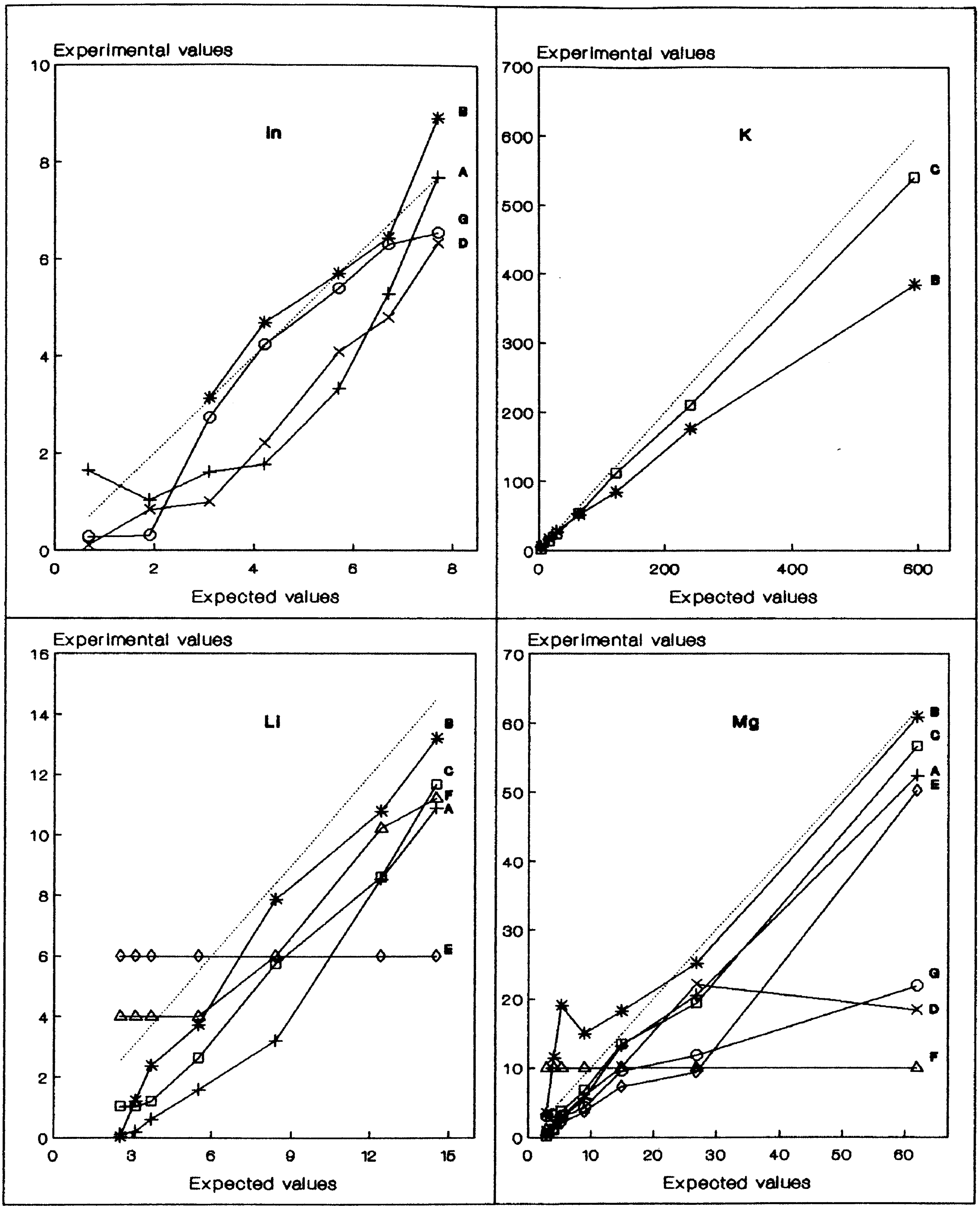
B
C
D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Experimental values
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C
B
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200
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Experimental values
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C
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9
12
15
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Experimental values
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C
A
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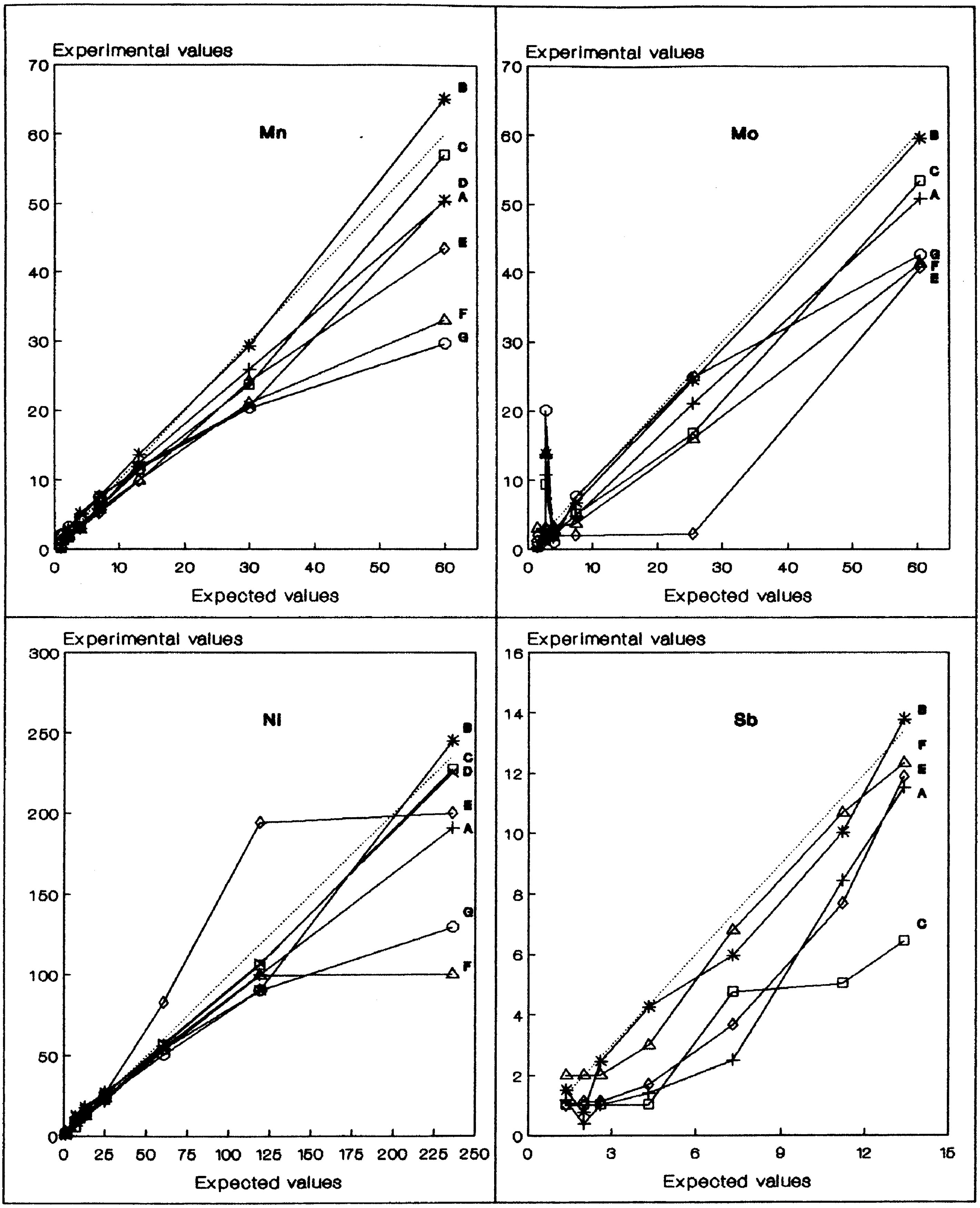
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50
60
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Experimental values
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40
30
20
10
0
Mo
B
C
A
G
F
E
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10
20
30
40
50
60
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Experimental values
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250
200
150
100
50
0
Ni
B
C
D
E
A
G
F
0
25
50
75
100
125
150
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200
225
250
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Experimental values
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14
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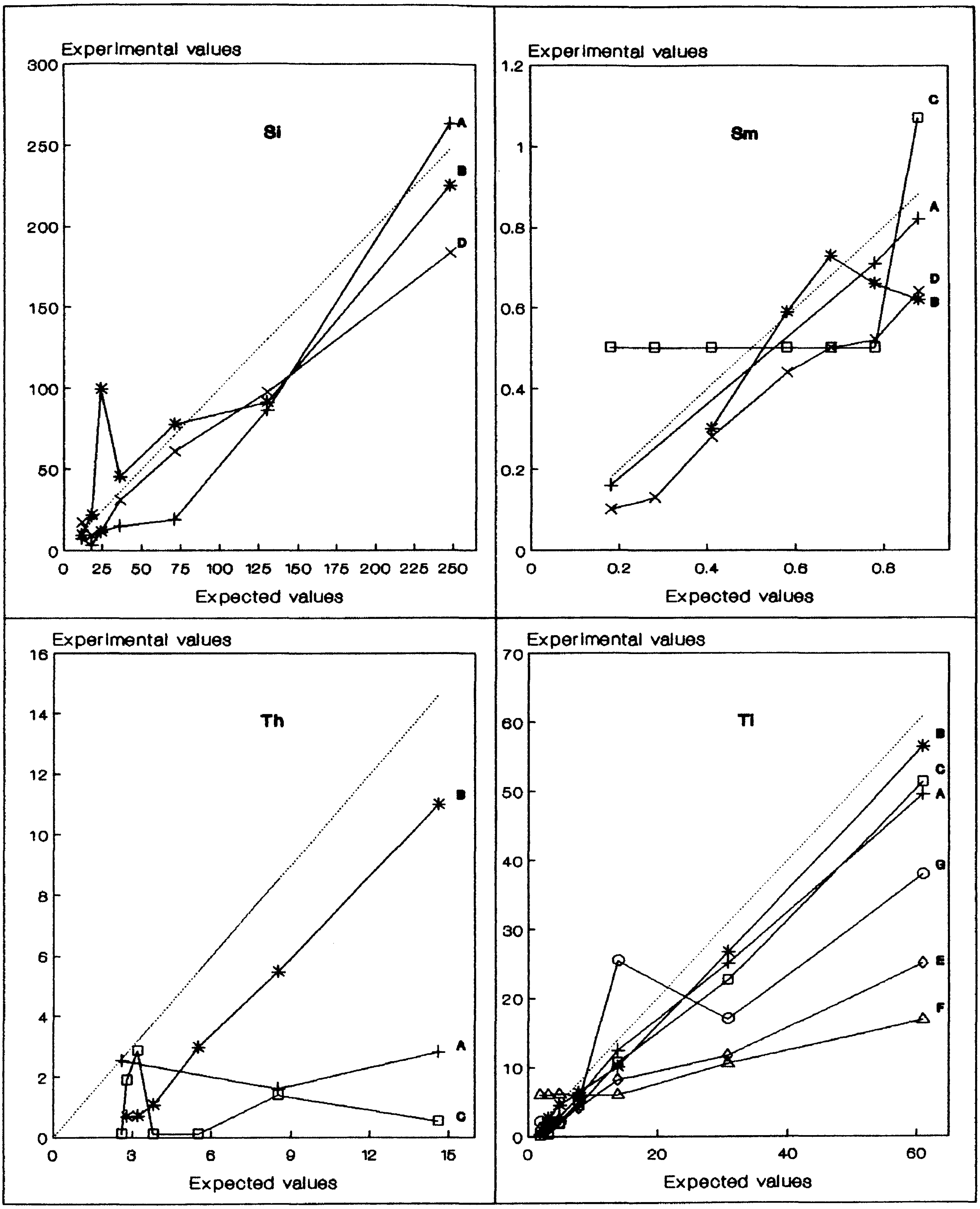
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D
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Expected values
Experimental values
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14
12
10
8
6
4
2
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Th
B
A
C
0 3 6 9 12 15
Expected values
Experimental values
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A
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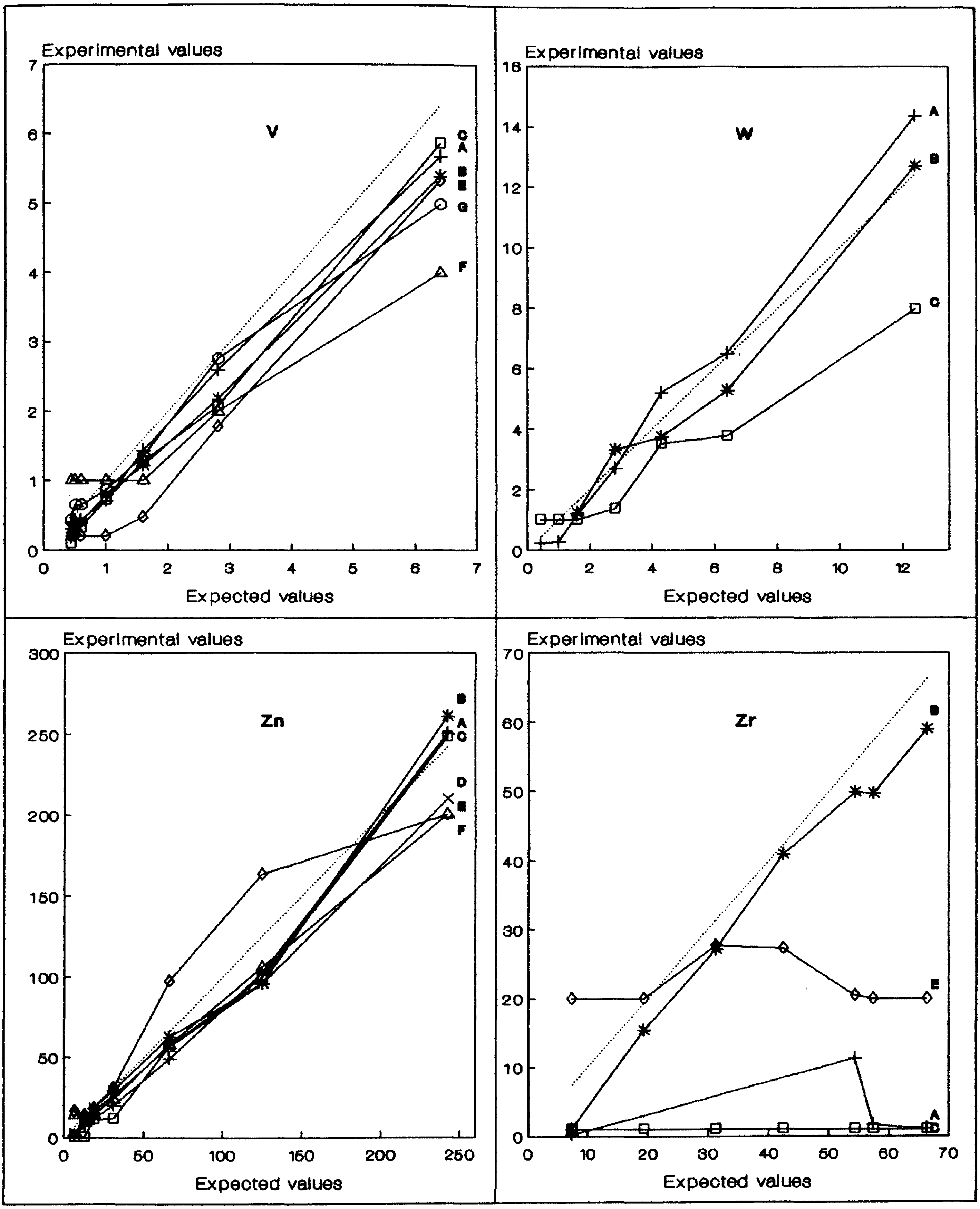
Expected values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5
6
7
Expected values
Experimental values
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14
12
10
8
6
4
2
0
W
A
B
C
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2
4
6
8
10
12
Expected values
Experimental values
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250
200
150
100
50
0
Zn
B
A
C
D
E
F
0
50
100
150
200
250
Expected values
Experimental values
70
60
50
40
30
20
10
0
Zr
B
E
A
D
0
10
20
30
40
50
60
70
Expected values

Dedicated to my wife

DENISE

and my children

GAVIN, NICOLE AND EDWIN

for their love, support and understanding

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SUMMARY

Spark-source mass spectrometry is used exclusively for the analysis of metal samples and other solid-state materials. Non-conducting powders are mixed with either silver or graphite as conducting medium, and pelleted into electrodes which are then mounted in the ion source. The dc-spark forms a plasma from which the ions are extracted and accelerated down a flight tube. The ion beam is defined by an electrostatic analyser and recorded on a photographic plate, after passing through a magnetic field which separates the ions according to their mass-to-charge ratio. The line blackening on the photoplate is measured using a microdensitometer. The data is interpreted using specialised computer software. A major advantage of photoplate detection in spark-source mass spectrometry is that the entire periodic table of elements can be recorded from a single analysis.

Reference standards are not available in South Africa for uranium compounds. A method of spiking the conducting material with trace impurities was developed after testing various graphite powders. Precision tests confirmed the homogeneity of the standards and the feasibility of using these for quantitative analyses. A comprehensive range of standards containing up to 34 elements, each using yttrium as an internal reference, were prepared and analysed quantitatively. A complete set of calibration graphs was compiled, providing relative sensitivity factors (RSF's) for these elements in a U_3O_8*/graphite matrix. For most of these elements, both the singly and doubly charged states were considered so as to obtain a correlation between the various ion yields. The accuracy obtained at a concentration level of 10 µg/gU is better than 20% for most of the elements determined. The* UF_4*/graphite matrix was also studied.*

This method was assessed by comparison with ICP, AA, spectrographic and spectrophotometric methods. Excellent agreement was confirmed.

KEYWORDS: spark-source mass spectrometry, U_3O_8*/graphite matrix,* UF_4*/graphite matrix, uranium compounds, relative sensitivity factors, photoplate detection, low-voltage discharge.*

OPSOMMING

Vonkbronmassaspektrometrie word uitsluitlik vir die ontleding van metaalmonsters en ander vastestofmateriale gebruik. Nie-geleidende poeiers word met silwer of grafiet as geleidende medium vermeng en in elektrodes gedruk wat dan in die ioonbron gemonteer word. Die gelykstroomvonk vorm 'n plasma waaruit die ione uitgeneem en in 'n vlugbuis versnel word. Die ioonbundel word deur 'n elektrostatiese analiseerder gedefinieer en op 'n fotografiese plaat opgeneem nadat dit deur 'n magneetveld beweeg het, waar ione volgens die massa-tot-ladingsverhouding geskei is. Die lynverswarting op die fotoplaat word deur 'n mikroverswartingsmeter gemeet. Die data word met gespesialiseerde rekenaarprogrammatuur vertolk. Die hoofvoordeel van fotoplaatdeteksie in vonkbronmassaspektrometrie is dat die hele periodieke tabel van elemente met 'n enkele ontleding opgeneem kan word.

Verwysingstandaarde van uraanverbindings is nie in Suid-Afrika beskikbaar nie. 'n Metode van toevoeging van spooronsuiwerhede tot die geleidende materiaal is ontwikkel nadat verskeie grafietpoeiers uitgetoets is. Presisietoetse het die homogeniteit en die bruikbaarheid daarvan vir kwantitatiewe ontledings bevestig. 'n Omvattende reeks standaarde met tot 34 elemente, wat elk yttrium as interne verwysing bevat, is voorberei en kwantitatief ontleed. 'n Volledige stel kalibrasiegrafieke is opgestel, wat relatiewe sensitiwiteitsfaktore (RSF's) vir hierdie elemente in die U_3O_8*/grafietmatriks verskaf het. Vir die meeste van hierdie elemente is beide die enkel- as dubbelgelaaide ladingstoestande beskou om 'n verband tussen die verskillende ioonopbrengste vas te stel. Die akkuraatheid wat by 'n konsentrasievlak van 10 µg/gU bereik is, is beter as 20% vir die meeste van die elemente wat bepaal is. Die* UF_4*/grafietmatriks is ook ondersoek.*

Die metode is deur vergelyking met IGP, AA, spektrografiese en spektrofotometriese metodes geëvalueer. Uitstekende ooreenstemming is bevestig.

SLEUTELWOORDE: Vonkbronmassaspektrometrie, U_3O_8*/grafietmatriks,* UF_4*/grafietmatriks, uraanverbindings, relatiewe sensitiwiteitsfaktore, fotoplaatdeteksie, laespanningontlading.*

CHAPTER ONE

INTRODUCTION

1.1 *Introductory review*

The double-focusing spark-source mass spectrometer Varian SM1B-F is well known for the analysis of trace impurities in solids such as conductors, semi-conductors and insulators. An electric discharge is generated between two electrically conducting electrodes which are made partly or wholly of the sample substance and mounted in a high vacuum. The electrode substance is evaporated and simultaneously ionised in the discharge. The ions emitted from this discharge are accelerated into the analyser, filtered according to their energy in the electrostatic analyser and analysed according to their mass-to-charge ratio, m/e, by deflection in the magnetic field. Ion-sensitive photographic plates are used to detect the ions and provide a permanent mass spectrum of the sample.

All elements with concentrations in the detection range may be analysed simultaneously in a single analysis. The complete mass range of interest is then recorded on a single photographic plate. This emphasises the selectivity and power of spark-source mass spectrometry in solid-state analysis. Very small sample sizes are required. The minimum mass of a non-conducting powder sample for a single analysis is only 0,1 grams which is then mixed with a conducting medium such as graphite powder. The physical size of a conducting metal or alloy sample for a single analysis is a piece one millimeter square with a ten millimeter length, which can be cut off from the bulk sample. The sensitivity with which a given element in a sample can be detected is in the same order of magnitude for almost all elements. Generally, it can be stated that the detection limit for almost all elements *is in the parts per billion (ppb) range. Some difficulties are, however, encountered in the quantitative determination of certain elements below the parts per million (ppm) concentration.*

If a sample has a completely unknown composition, the spark-source mass spectrum allows the analyst to carry out a quick and standard-independent survey of the composition of the sample, qualitatively or semi-quantitatively. This survey analysis provides the concentrations of practically all elements in the sample to as far down as the ppb range, with a deviation from the absolute value not exceeding at the most, a factor of 3. A major advantage in the analysis at trace levels is the fact that samples can be analysed without any preliminary chemical treatment. This eliminates possible direct, as well as indirect, sources of contamination.

For many of the analysis problems in industry, particularly in trace analysis, a qualitative or semi-quantitative analysis of the sample is sufficient. If, however, a greater degree of accuracy is required, then the amount of endeavour required to carry through an analysis is correspondingly higher and the duration of the analysis that much longer. It is then necessary to measure the transmission factors of the spectral lines of the elements of interest. Concentration values relative to the concentration of one or several internal or external reference elements are hence obtained. The precision which may be achieved using graphical evaluation methods is in the order of approximately 20 per cent.

The work involved in high precision analyses is more arduous and exacting. The analyst must rigorously apply a precisely defined method of analysis in the evaluation of photographically recorded *mass spectra. The large amount of spectral information must then be fully utilized [1]. This can be achieved only with computerised data interpretation methods. The program provides spectral line transmission values along with the necessary corrections such as isotope abundances, line surfaces, photographic sensitivity, background and loss of sensitivity of the photoplates through background [2].*

At present, the precision cannot be increased to values of better than approximately 20 per cent. This is largely due to the properties of commercially available photoplates. The statistical distribution of the silver grains on the photoplate surface as viewed through the microdensitometer slit gives the precision obtainable in mass spectrometric analyses of solids, an upper limit of 20 per cent. The percentage surface covering of the silver grains is a measure for the transmission factor for the relevant mass lines.

1.2 Motivation and scope of the thesis

Uranium compounds are produced to nuclear grade specifications by the Atomic Energy Corporation of South Africa Ltd. Maximum permissible levels are defined for a large number of elements in uranium oxide, U_3O_8. *The spark-source mass spectrometer and various other techniques and methods are used to analyse these compounds. However, these techniques have limiting factors, such as sample treatment, standard addition and spectral interferences, which are not applicable to the spark-source mass spectrometer.*

In order to perform quantitative analyses on the trace level impurities in uranium compounds, specifically U_3O_8 *and* UF_4, *making use of the internal reference standard method, the spark-source mass spectrometer first had to be characterised by deter-*

mining relative sensitivity factors (RSF's) for these impurities in the particular matrices.

At the start of this characterisation stage of the project, no suitable standards were available. The existing standards were incomplete in that they did not contain all the relevant impurity elements. The non-availability of international U_3O_8 *standard reference material (SRM) further complicated the situation. Due to these limitations, graphite standards containing all the required impurity elements were prepared.*

After this characterisation phase had been completed, the spark-source mass spectrometer was used to standardise a series of internal U_3O_8 *working standards. This technique can also be used in other applications in the nuclear industry where contamination must be controlled through a quality control programme.*

This investigation had as its aim to conduct a comprehensive evaluation of the method of relative sensitivity factors for the determination of trace elements in U_3O_8*. The project also afforded the opportunity to study the* UF_4 *matrix where the effects of an excess of fluoride ions in the plasma had a marked effect on the ions recorded on the mass spectrum. This part has been studied in lesser detail. The evaluations were carried out to a point where routine analyses could be performed on the basis of the documented procedures. It was of prime importance to incorporate safeguards for reliable data acquisition and interpretation when doing routine analyses. This thesis should serve as a useful reference manual for the application of spark-source mass spectrometry in the nuclear industry. It contains extensive guide-lines for spectrum identification in uranium oxide and fluoride matrices. Data for fluoride matrices has never been published in the open literature.*

CHAPTER TWO

THE FUNDAMENTALS OF SPARK-SOURCE MASS SPECTROMETRY

2.1 *The physics of plasma formation*

The most commonly used method of generating ions in the analysis of solids is with the radio frequency (RF) spark. However, this type of ion source has proved to be deficient in many respects as will be discussed below.

In the Varian SM1B-F spark-source mass spectrometer, the triggered low-voltage discharge (secondary spark) is used to generate ions. This low-voltage discharge is generated in turn by an external high-voltage impulse (primary spark) [3].

The major differences between the low-voltage spark and the RF spark can be summarized as follows:

The energy width of ions emitted from the triggered low-voltage discharge is much smaller than for the ions generated by the RF spark. This means that more ions pass through the entrance to the electrostatic analyser for the low-voltage spark. Due to this factor the time taken to determine an element in a sample at a given concentration with the same sample consumption is considerably reduced for the low-voltage spark compared to the RF spark.

When high-voltage electric spark-overs occur in the ion source due to too great a distance between the two electrodes, and also during the low-voltage discharge, some of the electrode substance is transferred from one electrode to the other. With the RF spark the polarity of the electrodes alters so that particles of *the electrode substrate flow in both directions. With the low-voltage discharge, the polarity of the electrodes does not alter, therefore during each discharge a new amount of the cathode is evaporated, partly ionised and condensed on the anode so that the volume of the anode increases and that of the cathode decreases. The flow of electrode substrate particles in the same direction eliminates the possibility of some components of the electrode substance becoming preferentially evaporated, a process which happens in the RF spark.*

The ratio of multiply charged ions to singly charged ions is not constant in the case of the RF spark. The constant ratio in the case of the low-voltage discharge offers an advantage in that the quantitative analysis of a sample is not restricted to evaluating lines of singly charged ions, but also multiply charged ions [1]. This is useful, especially in cases where the line of a singly charged elemental ion is interfered with by a line from another elemental ion such that the first element cannot be quantified. Then a multiply charged ion of the same element can be used to quantify.

Ions formed in the ignition phase (primary spark) of the impulse low-voltage spark exhibit characteristics making them unsuitable for quantitative analysis which resemble those obtained with the RF spark. By using time resolved mass spectrometry [4] with the SM1B-F, all these unwanted ions formed in the ignition phase are rejected and only ions generated during a selected burning time interval of the low-voltage discharge arc are allowed to pass through the mass spectrometer where they are analysed according to their mass-to-charge ratio and detected photographically.

Various processes occur between the two electrodes in the ion source. The electrode material is first evaporated/volatilised. Thereafter the vapour is selectively atomised and subsequently ionised [5, 6]. This resulting collection of charged particles is called a plasma. The above processes occur during the low-voltage arc discharges (secondary sparks) which are induced by high-voltage ignition pulses (primary sparks). Eventually the ions are accelerated into the mass spectrometer due to the 20 kV acceleration voltage. The plasma can thus be seen to be floating at this voltage. The formation of ions in this manner lead to ions found only in the elemental atomic stage. No molecular species are formed, except clusters which are formed due to recombinations within the plasma.

The primary and secondary sparks are controlled by pulse statistics and spark parameters. This means that the plasma created between the two electrodes in the ion source (and ultimately also the ion beam) can be controlled by the spark parameters.

Arc discharges are generated between the two electrodes in the ion source in order to evaporate the samples to be analysed. The spark repetition rate of individual discharges can be set in steps of 10, 30 or 100 Hz by adjusting the frequency. The voltage of this arc discharge is approximately 850 V and is set. Each discharge is induced by a high-voltage ignition impulse and subsequently maintained for a specified period of time as a low-voltage discharge with a constant current. This discharge current of the low-voltage arc can be set in 10 equal stages between approximately 3 and 10 A. The high-voltage ignition impulse used to induce discharges has a maximum ignition voltage of approximately 64 kV with +32 kV on the one electrode and -32 kV on the other electrode. The energy of the ignition spark can be set to 3 different intensities.

The above spark parameters are directly related to the results obtained in respect of atomisation and ionisation of the electrode material.

Ions generated during the burning interval of the discharge and subsequently accelerated into the flight tube of the mass spectrometer can be deflected in front of the entry slit. This means that ions are only allowed to reach the entry slit during a certain pre-selected time in the burning interval and the ion current is completely cut out during selected dead times (impulse statistics). In this way the ion beam can be controlled.

2.2 Mass spectrometer design features

A simplified block diagram of the Varian SM1B-F spark-source mass spectrometer is given in Figure 2.1. The instrument makes use of a triggered low-voltage direct current (d.c.) discharge in the ion source region where ions are generated. The ion beam then undergoes double-focusing on entering the analyser, comprising the electrostatic analyser (ESA) and magnetic sector with Mattauch-Herzog geometry. A photographic plate is used to detect the ions.*

The generation of ions in the ion source region of the mass spectrometer has been discussed in Section 2.1. All parts in close proximity of the actual spark i.e. the acceleration plate and the shield plate, are made of tantalum and can be cleaned easily by chemical or mechanical means. Electrical focusing is not possible because of the relatively large initial energy dispersion. The design of the ion source is therefore relatively simple, consisting only of the acceleration system and a deflection condenser.

** Varian MAT, now Finnigan MAT, GmbH, Postfach 14 40 62, D-2800 Bremen 14, Federal Republic of Germany.*

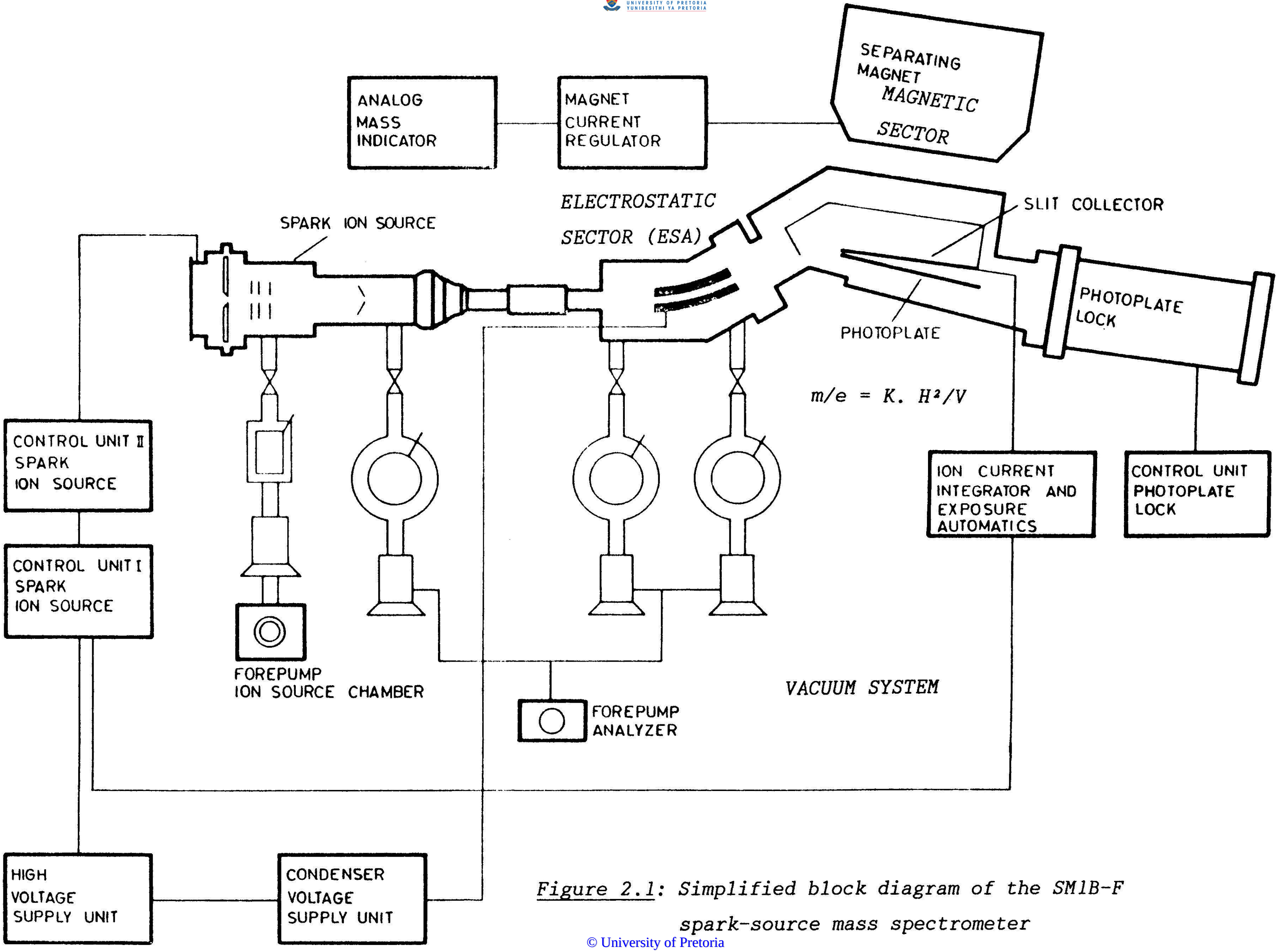

Figure 2.1: Simplified block diagram of the SM1B-F spark-source mass spectrometer

An important feature of the instrument is that all original tube electronic units have been replaced by units using solid-state electronic components. The vacuum system has also been updated. Two large turbo-molecular pumps are used to achieve a working vacuum of 10^{-4} Pa in the ion source region of the mass spectrometer. Two ion-getter pumps are used in the analyser region (electrostatic analyser (ESA) and magnetic sector) to obtain a vacuum down to 10^{-7} Pa. One small turbo-molecular pump is used to obtain a vacuum of 10^{-3} Pa in the photoplate lock.

The ion optical system of the SM1B-F mass spectrometer is given in Figure 2.2, which shows the path of the ion beam. In the ion source, particles of the substance to be investigated are ionised, accelerated through a system of electrostatic lenses by means of a stable 25 kV Spellman* high-voltage d.c. supply unit, and focused into a narrow beam. This ion beam must be so aligned that it hits the centre of the object slit (exit slit of the ion source). To achieve this, the ion source can be aligned in all three directions.

The object slit (entrance slit of the ion optical system) defines the width of the ion beam so that the desired resolution can be set. In order to meet the requirements of quantitative analysis and the separation of doublets, the ion source is equipped with a pair of slits having entry slit widths of 30 and 300 µm. With a slit width of 300 µm the aberrations of the ion optics is negligibly small. Since the slit is evenly illuminated at the same time, rectangular-shaped line blackenings are obtained with the wider slit width on the photoplate.

* Spellman High Voltage Electronics Corporation, Plainview, New York, 11803, U.S.A.

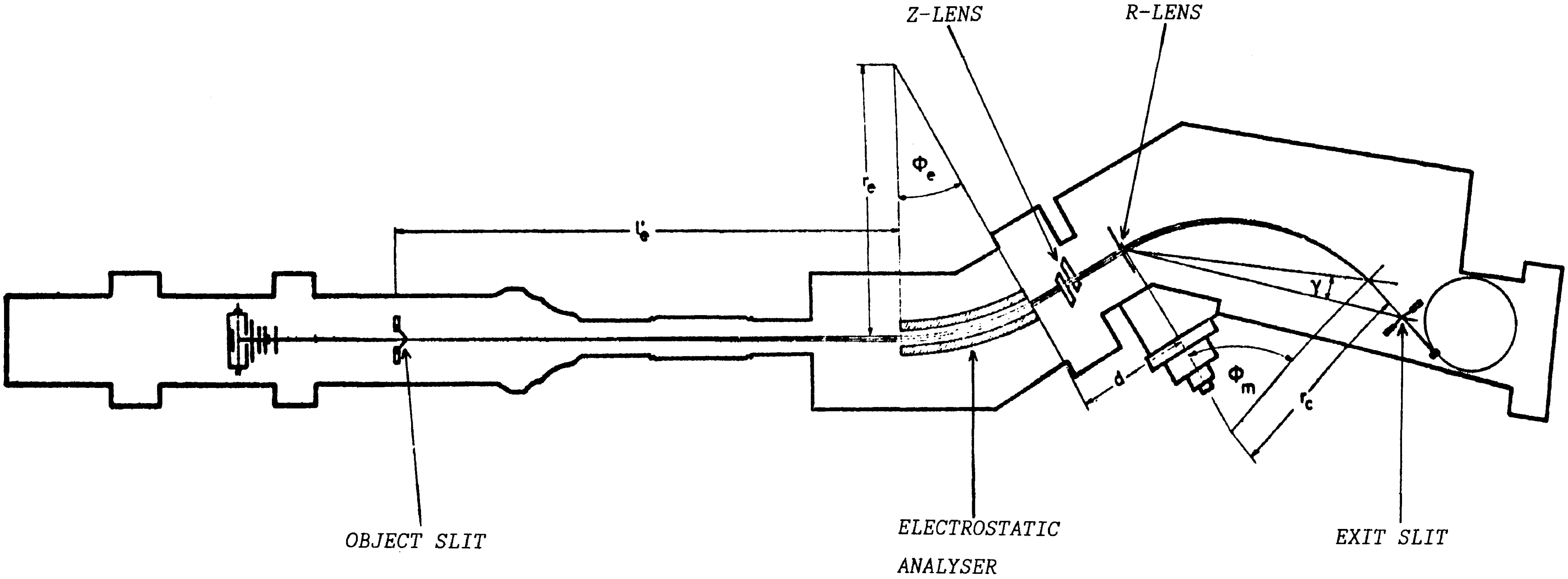

Figure 2.2: Path of ion beam through the SM1B-F spark-source mass spectrometer

The formula used to determine resolution (R) is given by:

$$R = \frac{M_o}{\Delta M}$$

where:

M_o is the nominal mass of the particular element, and
ΔM is the difference between the mass defect of the element under scrutiny and the mass defect of the interfering element (see also page 41).

The resolutional requirement is given in the fourth column of Appendix B on page 177. The resolving power is defined as that resolution required to resolve two mass spectral lines lying adjacent to each other as a doublet on a photoplate.

The resolving power of the SM1B-F mass spectrometer is up to 10 000 and depends on the position on the photoplate, the magnet strength setting as well as the object and exit slit settings. Practical resolving powers obtained during this investigation range between 2 000 and 5 000.

The electrostatic deflection field between the plates of the curved analyser produces an energy dispersion and a direction focusing. Ions of selected energy are thus directed in one parallel beam on emergence from the electrostatic analyser.

The potential difference between the ESA plates is kept very stable and is supplied by two 5kV Spellman high-voltage d.c. supply units. The energy band of ions leaving the ESA is defined by a narrow band within the Boltzman natural distribution of the energy population shown in Figure 2.3.

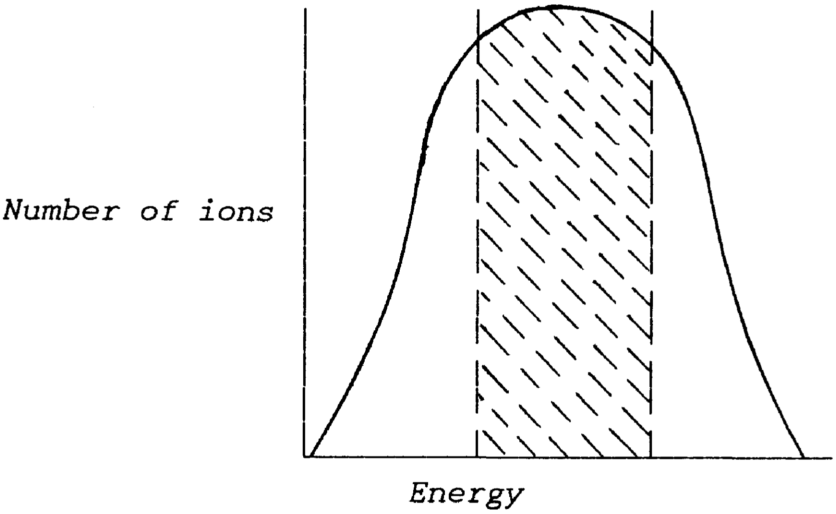

Figure 2.3: Shaded area represents energy band of ions selected on leaving the ESA

On leaving the ESA, the ion beam is defined vertically, called the z-direction. The direction of the ion beam emerging from the ESA can be controlled and correctly adjusted, so that the beam passes the monitor lens plates symmetrically and enters the magnetic field horizontally. The casing of the z-monitor acts as a shield against influences from the magnetic field as does the so-called Herzog lens. This lens creates a magnetic short circuit and ensures that the area within the z-lenses is not disturbed by the stray field of the separating magnet. At the end of the Herzog lens, the energy slit is mounted just in front of the magnet chamber. The energy-defining slit determines the point of entrance of the ion beam into the magnetic field and can be shifted horizontally, called the r-direction. The position of the ion beam can also be controlled in the r-direction prior to its entrance into the magnetic field. The path of the ion beam through the Herzog lens and z-and-r-monitors is shown schematically in Figure 2.4.

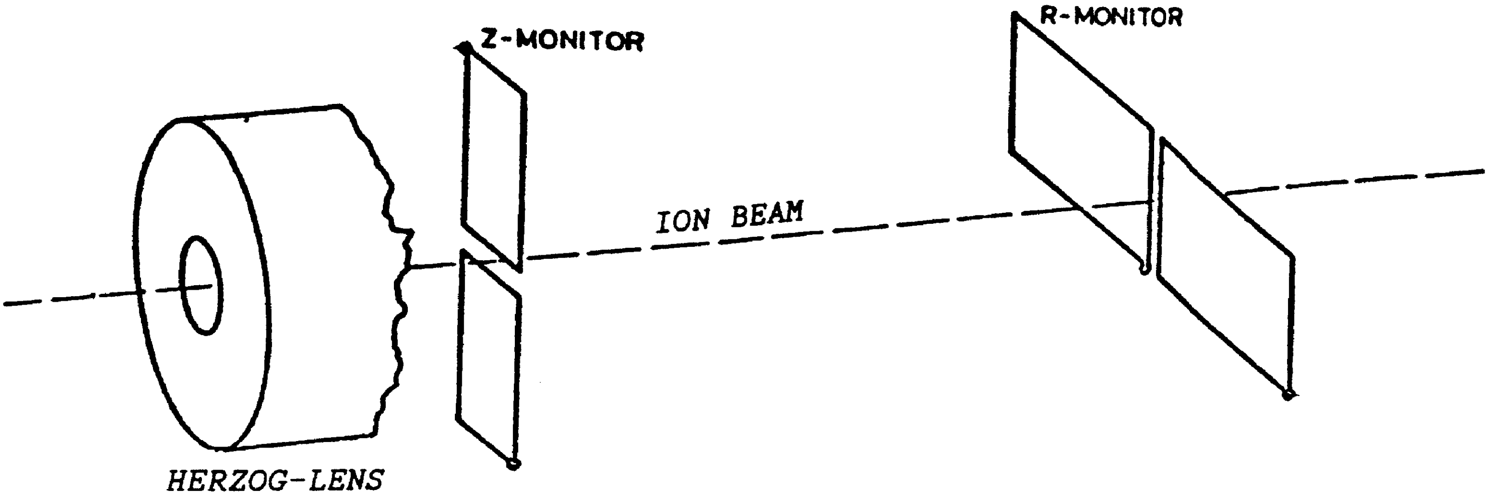

Figure 2.4: Path of ion beam through Herzog lens and z- and r-monitors

The ion beam, which is defined in the r- and z-directions, enters the magnetic field produced by an electromagnet, whose current is supplied by a stable solid-state magnet power supply unit. The double-focusing plane (the plane in which ions of equal m/e ratio are focused with respect to direction and energy) lies outside the magnetic field. Due to this location of the plane outside the field, it is possible to use a slit collector positioned in front of the photoplate for the measurement of the total ion current. The ions entering the magnetic field are bent according to their mass-to-charge (m/e) ratio and recorded on the photoplate.

2.3 Ion detection and measurement

In the quantitative analysis of solids, it is not only customary but necessary, in order to cover as large a concentration range as possible, to bring a staggered series of exposures of the same mass spectrum onto one photoplate. The selection of such an exposure pattern is discussed on page 21. Aspects of the ion-sensitive photographic plates are discussed on page 22.

Since the ion current emitted from the ion source fluctuates with time, a slit aperture detector is used to record a fraction of the total ion current. This ion current is integrated over time to provide a measure of the total ion current falling onto the photoplate during each exposure.

In the SM1B-F spark-source mass spectrometer the electrodes of the slit aperture detector are positioned directly in front of the photoplate, i.e. at the exit boundary of the analyser's magnetic field. The ion current integrator permits the exact measurement of the charge down to 0,01 picocoulomb (pC).

There are a number of publications in existence on general measuring techniques used in conjunction with double-focusing mass spectrometers with a spark-source [1]. The measuring technique used in this work required specialised hardware and software

[7, 8] specifically designed and developed to evaluate spectral lines on ion-sensitive photoplates.

Besides photoplate recordings, ions can also be recorded with an ion collector utilizing a Faraday cage or a secondary electron multiplier (SEM) as electrical detection systems. Two focusing plates positioned behind the exit slit direct the ion beam onto the ion collector. Further plates located in front of the exit slit are connected to a saw-tooth generator. The ion beam can therefore be made to pass at intervals before the slit. Connected to the SEM of the ion collector, the ion beam can be displayed as a peak on an oscilliscope screen. Alternatively, the ion beam can be recorded with a Faraday cage which can be exchanged for the SEM.

The SM1B-F spark-source mass spectrometer used by this laboratory does not make use of electrical detection as this facility has been removed from the instrument.

The advantages of utilizing photoplate detection can be summarized as follows:

Photographic plates provide a permanent record of the spectrum obtained for a sample. Once the analyst has analysed the photoplate, it can be stored and re-used at a later stage to obtain additional information. The complete spectrum of impurity elements present in the sample is obtained on a photoplate. This helps the analyst when eliminating possible interferences on a specific spectral line.

Sophisticated hardware and software exist for the reading and interpretation of mass spectrographic ion-sensitive photoplates. The sensitivity of the emulsion layer on Ilford Q plates meets the requirements for the detection of ions of low concentration levels.

CHAPTER THREE

EXPERIMENTAL

3.1 *Mass spectrometer operation*

3.1.1 *Operation of the instrument*

The operation of the instrument, from the time the sample is loaded in the ion source of the mass spectrometer until the photoplate has been exposed and removed to the dark room for development, is comprehensively described in the operating manual [9] and will not be repeated in this thesis.

3.1.2 *Preparation of electrodes*

Solid-state compounds which are analysed with spark-source mass spectrometry can be divided into two groups: The first group, metals and alloys, are electrically conducting and analysis can be performed directly on a piece of the material. The second group, powders, can be divided into conducting and non-conducting materials. For powder samples, electrodes have to be pelleted. However, for non-conducting powders, a conducting medium such as silver or graphite must first be mixed with the sample before electrodes can be pelleted.

For non-conducting powder samples, these are first ground using an agate mortar and pestle to ensure homogeneity of the sample. Thereafter, the sample is weighed and combined with graphite in the appropriate dilution ratio, using yttrium as an internal standard. The preparation of graphite standards and the use of yttrium as an internal standard are discussed on pages 26 and 28, respectively.

Two or three glass beads are then placed into the polyethylene vial with the sample/graphite mixture to promote good mixing using a Retsch[*] Type MM2 agitator/mixer or a Wig-L-Bug[#] mixer, serial no. Y56737. A cylindrical high-density polyethylene pill (called a slug), with two holes through it, is then placed into a stainless steel holder. This holder is specially manufactured to accommodate the pill and also has a sample loading facility. Using a small spatula, the sample mixture is carefully inserted into the holes of the pill through the sample loading facility of the holder. A plunger is used to compact the sample. The exercise requires gentle action in order to produce an electrode. The pill is then placed in a die and compacted to 22 - 25 tons using a Spex[@] Industries 25 ton hydraulic bench press. The pill is subsequently placed on a perspex support and a stainless steel plunger is used to press out the two electrodes. The tips of each electrode are carefully broken off to expose a representative new surface for analysis. The electrodes are finally clamped in tantalum electrode holders and mounted in the ion source of the mass spectrometer.

3.1.3 *Spark generator parameters*

It was important in this investigation to keep all the instrument parameters constant throughout the experiments so as to eliminate possible differences from one photoplate to the next. However, as a result of the wide concentration range employed in the graphite standards, certain parameters were changed slightly to suit the particular analysis. The various instrument parameters are given in Table 3.1.

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[*] *F. Kurt Retsch KG, 5657 Haan, Neuer Markt 25, Germany.*

[#] *Wig-L-Bug, Crescent Dental MFG. Co., Chicago, Illinois, 60616, U.S.A.*

[@] *Spex Industries Inc., Metuchen, N.J., 08840, U.S.A.*

Table 3.1: Instrument parameters

Vacuum conditions:	
Electrostatic analyser	10^{-6} Pa
Magnetic analyser	10^{-7} Pa
Ion source (when sparking)	10^{-4} Pa
Photoplate lock	10^{-3} Pa
Slit settings:	
Object slit width	10 - 20 μm
Analyser entrance slit width	0,6 mm
Energy-defining slit width	0,8 mm
Potentials:	
Ignition spark voltage	32 kV
Low d.c. discharge voltage	850 V
Electrostatic analyser voltage	± 750 V
Accelerating voltage	± 20 kV
Magnet settings:	
Magnetic field	14 000 Gauss
Magnet current	4,6 A
Mass range covered	5 - 165 Daltons
Spark parameters:	
Low voltage discharge current	2 - 4 A
Spark pulse duration	20 μsec
Spark pulse repetition frequency	30 Hz
Ignition voltage intensity	Medium (No 2 setting)

It is imperative to wait until the desired vacuum has been reached in the various sections of the mass spectrometer before starting with the analysis. Poor vacuum conditions could cause short circuiting in the ion source region and vacuum banding across the photoplate in the magnetic analyser region.

The various slit width settings of the mass spectrometer were unchanged throughout the investigation. The ignition spark and low d.c. discharge voltages were also kept constant. These two potentials are set and fixed in the pulse statistics unit. The electrostatic analyser voltage could be changed with a 2 - 3 volt tolerance, but the positive and negative voltages were kept in perfect balance so as not to deflect the ion beam passing through the two slits. The accelerating voltage could also be changed with a small tolerance as it was used to direct the ion beam through two ion source slits in order to balance the ion beam monitors.

The magnet settings of the mass spectrometer were kept constant throughout an experiment to ensure that the various exposure spectral lines were directly aligned beneath each other on the photographic plate. Adjustments can be made on the microdensitometer to correct skewness which results from slight misalignment of the photoplate mounting in the detection compartment.

Most of the spark parameters, as set out in Table 3.1, were kept constant. The spark pulse duration was fixed in the pulse statistics unit, whereas the other settings could be set externally. Whenever very short exposures were required, especially for samples with high concentration levels of impurity elements, use was made of beam chopping whereby only certain portions of the ion beam were allowed through the lenses, making it easy to capture short exposures on the photoplate. The low-voltage discharge current was constantly changed in order to maintain the ion beam. This parameter has a direct influence on the ionisation that is taking place within the plasma generated in the ion source.

The polarity configuration of the two electrodes mounted in the ion source depends on the type of sample. The ion current differs from a metal sample to a powder sample. In order to achieve the optimum ion current the polarity must be changed to suit the sample type.

Possibly the single most important setting that must be constantly adjusted throughout an analysis is the spark gap between the two electrodes. The position of the two electrodes relative to the aperture of the ion source is also very critical. The positioning of the two electrodes during sparking is directly related to the ion current monitored. This spark gap must be kept constant throughout the analysis by repeated resetting of the gap as the electrode material is being depleted.

3.1.4 Exposure pattern selection

The exposure pattern to be used to analyse a sample depends on the concentration range of impurity elements present. The ion beam is recorded as a charge which is measured in picoCoulombs (pC). For unknown samples, a standard exposure pattern is implemented. However, for samples which have very high concentration levels of impurity elements, very short exposures must be selected to be able to obtain a workable transmission curve. Similarly, for samples that have very low concentration levels of impurity elements, very long exposures are needed to detect these low concentrations. The exposure pattern is based on a natural logarithmic scale due to the large range of the exposures (one to 20 000 pC). Three exposure patterns were compiled to cater for the range of graphite standards prepared. These standards and preparation methods are discussed on pages 26, 103 and 122. The U_3O_8 sample used for the acquisition of the blank data required a very long exposure pattern.

There are normally 32 positions which can be utilized on a photographic plate. The analysis time is totally dependent on the exposure pattern selected. For an exposure pattern of up to 20 000 pC, the average analysis time is of the order of two hours, depending on the spark parameters. However, replacing short exposures by long exposures, to ensure detection of very low concentrations, increased the analysis time up to seven hours using the same ion current and sparking parameters. Exposure patterns should be chosen in relation with the lifetimes of electrodes.

3.1.5 Detection

Ion-sensitive photographic plates Ilford* Q plates, are used in the photographic detection system [10].

Silver bromide (AgBr) crystals embedded in a gelatine matrix, which is the emulsion layer covering the glass plate, are reduced to metallic silver (Ag) during the development stage. This takes place on the photoplate only where ions from impurity elements in the sample have fallen, forming clusters of silver atoms, called latent image centres. During the fixation stage, the remainder of the AgBr crystals are removed, leaving only the characteristic spectral lines on the emulsion with varying degrees of blackening, according to the exposure pattern and concentration of impurity element ions. The developing procedure for these Q plates is a standard method [7]. Whenever a photoplate

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* Ilford Limited, 14 - 22 Tottenham Str, London, W1POAH England.

has to be developed, it is a cardinal rule that fresh solutions of developer and fixer must be used. This is necessary to eliminate the possibility of under-developing the photoplate and also to remove all of the residual silver halide crystals so as to have a clear background transmission of light on the photoplate. A hardener is also added when rinsing the photoplate off, to aid image formation.

Hereafter, the photoplate is placed in a specially designed water tower with running demineralised water for half an hour. This step ensures that no fixing agents remain on the photoplate which, with time and light, darkens the background emulsion. A wetting agent is finally added which aids rapid and uniform drying. The glass side of the photoplate is then dried off and the photoplate placed in a specially designed dust-free black box where the emulsion is allowed to dry before the photoplate is inspected under the microscope. It is very important to follow the standard developing procedure so as to minimise differences in photoplate data due to differences in the photographic development procedure. The sensitivity of the photoplates in a particular batch is very similar. Slight variations do not influence the results as an internal reference standard normalises the data.

3.2 Preparation of Standards

3.2.1 Reagents

The reagents used to prepare the standards consist of two parts, namely the graphite powder and the solution containing the impurity elements of known concentration.

Various graphite powders were evaluated for this application. The most important consideration was the number of and concentration levels of impurity elements present. Graphite powder with the least background spectral lines should be selected to act as conducting medium in the spark-source mass spectrometer. Another prerequisite was that the powder should be wettable and pelletable, wettable in the sense that it would be able to adsorb drops of the standard solution and pelletable in the sense that electrodes could be pressed from the graphite powder. Ringsdorff[*] spectrographic powder, Grade RW-A, has very good pelletability, but is not very compatible with an aqueous solution. Another graphite powder tested was a French spectrographic carbon Ref 9900-208-I7 387, from Le Carbone[#], which was also not wettable. The only two graphite powders suitable were a spectroscopic powder from Union Carbide Corporation[@] (UCAR), Grade SP-1, Lot Number B92, Catalogue No. L 4100, and an Ultra 'F' purity electrode graphite from Ultra Carbon Corporation[$], Material UCP-1-200 powder, Lot Number 112-6-37. The Ultra 'F' graphite formed pellets (electrodes) which produced a better ion signal and had a cleaner background spectrum than UCAR SP-1 graphite, although it was slightly more difficult to wet. Both, however, were most suitable graphite powders to use in preparing standards.

The choice of impurity elements in U_3O_8 matrix was limited to those listed for nuclear grade specification for trace impurities

[*] Ringsdorff Werke, GmbH, Bad Godesberg - Mehlem.

[#] Le Carbone, Lorraine, Paris, France.

[@] Union Carbide Corporation, Carbon Products Division, New York, N.Y., 10017, U.S.A.

[$] Ultra Carbon Corporation, P.O. Box 747, Bay City, Michigan, 48706, U.S.A.

in uranium reactor fuels. The choice of impurity elements in a UF_4/graphite matrix is discussed on page 81. Impurity elements whose isotopes interfered with other element isotopes in such a way that they could not be measured, could not be evaluated using this method.

It was possible to obtain Spex* custom plasma standard solutions with concentrations of either 1 000 or 10 000 µg/ml for most of the selected impurity elements which are used in inductively coupled plasma (ICP) optical emission spectroscopy. These standards are referred to as "ICP standards" in the text below. It has been shown that the relative sensitivity factor for an impurity element is the same irrespective of a nitrate or oxide matrix [11]. Appropriate volumes of the standard solutions were added together to form a solution containing all the impurity elements, which was subsequently added to the graphite powder to prepare standards.

A set of Spex* diluted powder standards, denoted G-7, containing 49 common elements over seven concentration ranges using In as internal standard, were also analysed with base U_3O_8 material which contained very low levels of impurities (see Table 5.1 on page 106). These standards were found unsuitable for a number of reasons, of which the most important is their inhomogeneity. The concentration of the internal standard, In, is also too high for spark-source mass spectrometry applications. The powder does not form suitable electrodes when pelleted.

* Spex Industries Inc., Metuchen, N.J., 08840, U.S.A.

3.2.2 Preparation of standards in a graphite matrix

The desired volume of a specific ICP standard was chosen depending on the final concentration and the total mass of graphite standard required. The approach is demonstrated by the following example:

- Final concentration of graphite standard for element X relative to uranium: 10 µg X /gU.
- Concentration expressed relative to graphite: 40 µg X /gC (ratio of U to graphite is 4:1).
- Total mass of graphite standard required: 5 grams.
- Concentration then becomes: 200 µg X /5gC.
- Concentration of ICP standard: 1 000 µg X /ml.
- Expressed in microlitres : 1 000 µg X /1 000 µl.
- By extracting 200 µl from the ICP standard, the required concentration of 200 µg X /5gC is obtained.

The above procedure was adopted for each of the graphite standards prepared with the concentration range given on page 103 for U_3O_8, and on page 122 for UF_4.

Approximately 1 ml of a 1 000 µg/ml ICP standard for the various elements of interest was obtained in a clean pill vial. The necessary volume for each of the graphite standards was extracted from the pill vial using an appropriate Eppendorf* Varipette and placed carefully in a clean 50 ml Erlenmeyer flask containing deionised water and methanol (which was used to break the surface tension of the resultant solution). The concentration levels of impurities in the methanol were very low. Pb and Sn are the only elements which could interfere with the spectrum interpretation (see page 51). This procedure was followed for each of the

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* Eppendorf Gerätebou, Netheler & Hinz, GmbH, Postfach 65 06 70, 2000 Hamburg 65, Germany.

impurity elements, each time using a clean nib on the varipette.

Five grams of graphite powder was weighed off into a clean platinum crucible large enough to take the volume of graphite, using a clean stainless steel vibration spatula and a Mettler H10T mass balance.*

The wet doping technique was used to prepare the graphite standards. The standard solution is added to the graphite powder using a clean dropper until the powder is uniformily wet. Great care must be exercised when doing the addition, so as not to get any of the solution against the sides of the platinum crucible, as this could result in selective crystallisation during drying. The crucible is then placed under a 250W infrared lamp for about 20 to 30 minutes to dry the powder before the next addition is made. In total 15 to 20 such additions of the standard solution are made to the graphite powder with repeated washing down of the flask sides with a 30% methanol solution to ensure complete transfer from the flask to the platinum crucible. A glass rod is used after each drying to break up any lumps or crust that may have formed in the graphite powder and to mix the powder, in order to promote homogeneity. Once the standard solution has been completely transferred to the graphite powder, it is then dried in a vacuum oven at 80°C for 48 hours. After cooling down, the graphite standard is carefully transferred from the platinum crucible to a pill vial and capped. During the evaporation stage under the infrared lamp, the crucible is covered with a large-enough watchglass so as to prevent contamination from dust.

* *Mettler Analytical and Precision Balances, CH-8606, Greifensee - Zurich, Switzerland.*

3.2.3 Internal Standard Method

The general method used to quantify an unknown sample is to use the same photoplate for both the sample and a relevant standard [12]. In this way one eliminates slight differences from one photoplate to the next, e.g. photoplate response, differences in development, etc. A deciding disadvantage of such a method, especially if the sample turnover is great, is that the standard material becomes depleted. The time it takes to analyse both sample and standard is also impractical, especially when pump-down time is also taken into account. For these reasons, the use of an internal standard [13, 14] is far more desirable.

Yttrium (Y) was included in the preparation of graphite standards as an internal reference standard whereby differences between photoplates could be monitored.

The choice of Y as an internal standard was based on the following properties:

- it is an element which is not present as an impurity in nuclear fuels;
- both the 1+ and the 2+ spectral lines fall within the mass range of interest;
- Y is a mono-isotopic element having a mass-to-charge ratio of 89 in the singly charged state and 44,5 in the doubly charged state.

The general formula used to express a relative sensitivity factor (RSF), as shown by equation (3) on page 99, is reproduced to include Y as the internal standard (IS):

$$RSF = \frac{\dfrac{Q_x}{\bar{Q}_y}}{\dfrac{C_y}{C_x}}$$

where:

$\bar{Q}_y$ is the mean exposure value of Y for the charge states 1+ and 2+, C_y is the concentration of the internal standard Y added to the graphite standards, Q_x is the exposure value at 50% transmission of element X, and C_x is the concentration of an element X.

It can be shown, statistically, that it is advantageous to use the mean exposure value of two charge states, $\bar{Q}_y$, when expressing an impurity element's exposure value relative to the internal standard, Y.

The internal standard is also used as a control for photoplate evaluation and possible rejection by using the ratio between singly and doubly charged species as well as the mean exposure value between singly and doubly charged species, $\bar{Q}_y$. It has been found for Y in a U_3O_8/graphite matrix that the Y^+/Y^{2+} ratio lies between 3 and 4, with an average of 3,56 determined over 30 photoplates (n = 30). For a UF_4/graphite matrix the Y^+/Y^{2+} ratio lies between 1 and 2, with an average of 1,57 determined over 46 photoplates (n = 46). The mean exposure value, $\bar{Q}_y$, for Y in a U_3O_8/graphite matrix can be coupled to the Y concentration in the following manner:

80 µg Y /gC : $Q_{\bar{y}}$ = 4 895 where n = 31
60 µg Y /gC : $Q_{\bar{y}}$ = 7 098 where n = 14
40 µg Y /gC : $Q_{\bar{y}}$ = 9 384 where n = 12
20 µg Y /gC : $Q_{\bar{y}}$ = 20 066 where n = 37

The $Q_{\bar{y}}$ value for Y in a UF_4/graphite matrix is $Q_{\bar{y}}$ = 1 386, determined over 46 photoplates, and the Y concentration 100 µg Y/gC.

These values of Y^+/Y^{2+} ratio and $Q_{\bar{y}}$, for both U_3O_8 and UF_4 matrices, have been determined over a period of 10 months as the value of n indicates, and can be used to control the quality of analyses. Possible reasons for photoplate rejection are that the photoplate has not been developed properly, or that the sparking conditions used to analyse the sample are inadequate, or general instrument problems. This quality assurance approach is a new contribution to the methodology of spark-source mass spectrometry.

3.3 *Sample preparation:dilution ratio's*

Uranium compounds such as U_3O_8 and UF_4 are electrically non-conducting. For spark-source mass spectrometry analysis these have to be mixed with a conducting medium such as graphite or silver. The ratio between the conducting medium and the uranium compound determines the yield of impurity element ions. The mixing ratio depends on the conductance of the sample and is not subject to any generally applicable ruling.

Tests were conducted using different mixing ratios of Merck* nuclear grade U_3O_8, LAB 6344513, and graphite powder, as well as for a stoichiometric UF_4 sample and graphite powder. The number of mass spectral lines on the photoplate, using the appearance level method, was counted for the same element isotopes and charge states using different dilution ratios of sample to graphite. This method is based on the number of spectral lines which can be observed on a photoplate according to a specific exposure pattern for a particular impurity element, and is discussed on page 132.

For UF_4, it was found that a ratio of 1:1 between UF_4 and graphite by mass, yielded the most lines for the majority of the elements selected. Ratios up to 5:1 for UF_4 and graphite by mass were also analysed, yielding fewer lines for certain elements.

For U_3O_8 it was found that a ratio of 5:1 between U_3O_8 and graphite, by mass, yielded the most lines for most of the elements selected. Ratios from 1:1 for U_3O_8 and graphite, by mass, were also analysed. These ratios yielded fewer lines for all of the elements. The ratio of 4:1 for U_3O_8 and graphite by mass yielded for certain elements more lines than for a ratio of 5:1. The ratio of 5:1 between U_3O_8 and graphite implies a ratio of 4:1 between uranium (U) and graphite by mass as there is approximately 85% U in U_3O_8. When preparing electrodes with U_3O_8 and graphite the ratio of 5:1 by mass was used.

The different optimum dilution ratios between U_3O_8 and UF_4 can be ascribed to the fact that these compounds have different matrices resulting in different plasma conditions.

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* E Merck, Frankfurter Strasse 250, D-6100 Darmstadt 1, Federal Republic of Germany.

3.4 Data acquisition and processing

3.4.1 Microdensitometer

Once mass spectral lines have been identified on the photoplate as being solely representative of a particular impurity element in the sample, data capture is performed using a computer-controlled microdensitometer*, Model MD 100 [15]. Operating procedures are fully documented [16]. Data acquisition is performed using a Zenith# Data Systems microprocessor with dual auxiliary floppy disk drives, colour monitor and an OKI@ Microline 292 printer.

The microdensitometer settings are as follows:

Slit width	15 µm
Slit height	1,0 mm
Scanning speed	1,0 mm/sec

These settings are fixed from the outset and are determined by the characteristics of the spectral lines on the photoplate with regard to width and height.

* VEB Carl Zeiss JENA, DDR.

\# Fabriqué Par, Zenith Radio Corp., Springfield, Missouri, 65801, U.S.A.

@ OKI Electric Industry Co. Ltd., Tokyo, Japan.

The basic function of the microdensitometer is to measure the percentage light from a photocell that passes through the mass spectral line on the photoplate. The 100% setting is done using two clear plate regions at the low and high mass ends of the photoplate. It is thus imperative that all the emulsion is removed from these two regions. Transmission curves are drawn up from these transmission values used on the mass spectrometer. A limiting factor with the standard microdensitometer software is that the data manipulation matrix is dependent on the number of exposures utilised and the number of spectral lines to measure. The large number of impurity elements in a U_3O_8*/ graphite matrix, and the fact that some elements were measured both in the singly and the doubly charged state, created the need to compile two matrices.*

The most time consuming exercise is the preliminary setting up of the microdensitometer. This includes photoplate alignment on the carriage, obtaining relevant spectral line co-ordinates and the setting of windows around doublets and triplets. The last task is of utmost importance, especially for elements that occur only as doublets or triplets. This is discussed on page 45 for magnesium in a U_3O_8*/graphite matrix.*

The actual data acquisition is done rapidly, with the x- and y-motor drives activated under computer control. After each scan, the analyst must ensure that the y-motor has moved the carriage accurately from the preceding spectral line to the next and that the slit is correctly positioned over the spectral line on the photoplate. In this way, all the exposure spectral lines are scanned for the composition of a transmission curve.

The background noise correction transmission value is of extreme importance, especially for very light spectral lines. This value is subtracted from the emulsion background transmission which is measured on either side adjacent to the relevant spectral line of interest. If this background noise correction value is too high, it will result in the corrected emulsion background value being lower than the actual spectral line transmission value. This exposure point will then be rejected from the transmission curve.

Various factors affect the background noise correction value, amongst others, dust on the photoplate and ordinary electronic noise. The electronic units have to be kept well ventilated because if the analogue-to-digital converter gets warm, the background noise correction value becomes too large to work with. Ideally, this value should fall between 2 - 4%.

The data acquired is stored on floppy disk for further reduction and interpretation.

3.4.2 Linearisation functions

A second microcomputer and data processing software [7] are used for the data reduction and interpretation. The analyst is required to quantitatively determine the composition of the sample from the blackening of the mass spectral lines on the photographic plate. Plate blackening, which is measured by the light transmission through the emulsion, is not linearly related to the number of ions striking the emulsion. The plot of plate blackening against the natural logarithm of the number of ions striking the emulsion is an S-shaped curve dependent upon exposure conditions, ion momentum and plate development technique and is called the emulsion response curve or transmission curve.

The transmission curve is first investigated for possible outliers. Ideally, the curve should have a shape as in Figure 3.1 where there are a few saturated points as well as a few light points. The correct exposure pattern selected will ensure that such a transmission curve is obtained.

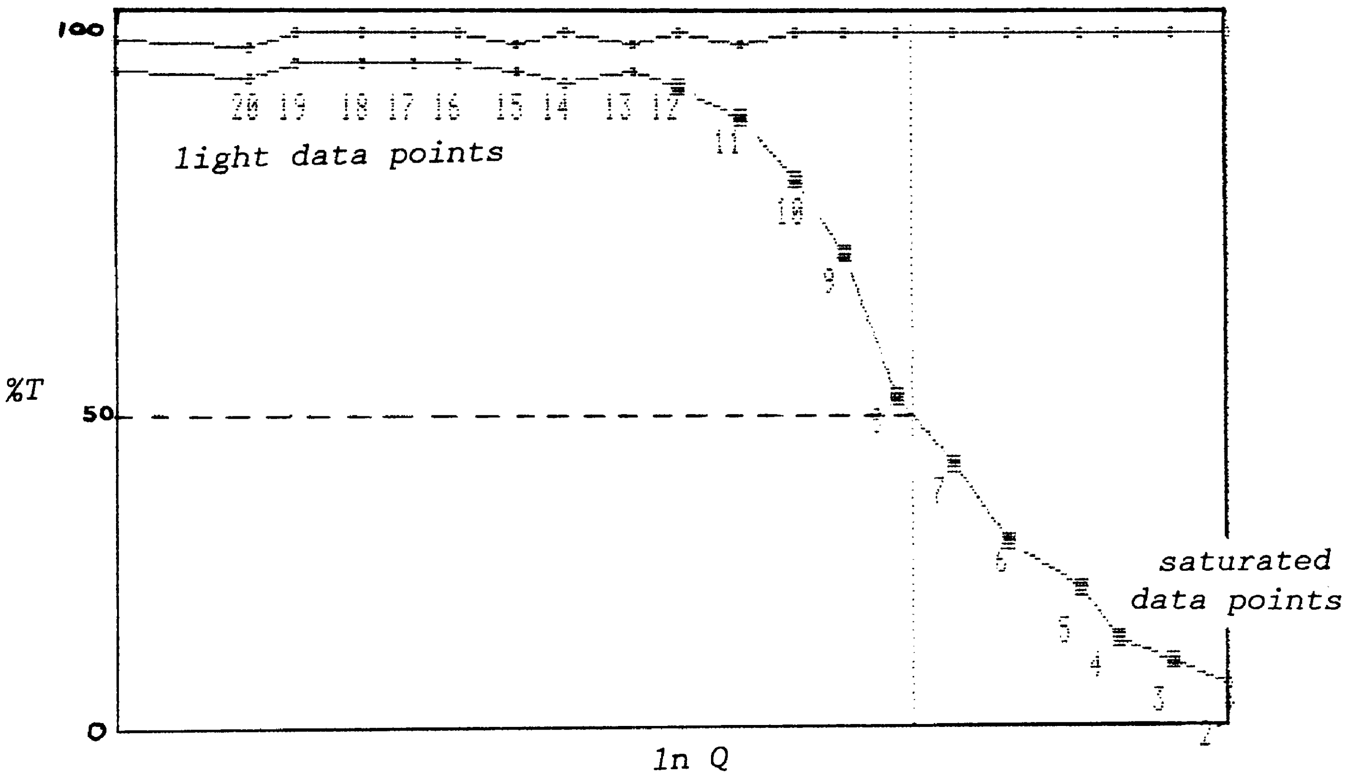

Figure 3.1: Typical good quality transmission curve

Transmission curves were linearised using the Hull function [8, 17]. Other functions that can also be used are the Seidel and Wagner functions [7]. However, these are more applicable to special applications and were not employed for this investigation. Although the semi-empirically derived Hull formula is not universally suitable for treatment of all data, it represents an approach which is adequate, provided that the exposure range is appropriate to the concentration of the particular element under investigation. For the Hull function plot, a gradient after linearisation of between 0,7 and 1,7 is acceptable. Points far outside the effective range for the Hull function were removed. Transmission values between 10 and 75% best fitted the Hull function, providing straight lines having correlation coefficients near unity. This is best illustrated in Figure 3.2. The final choice of acceptable data points for the Hull function plot depends on the assessment of the analyst and is based on experience rather than on any firm statistical approach.

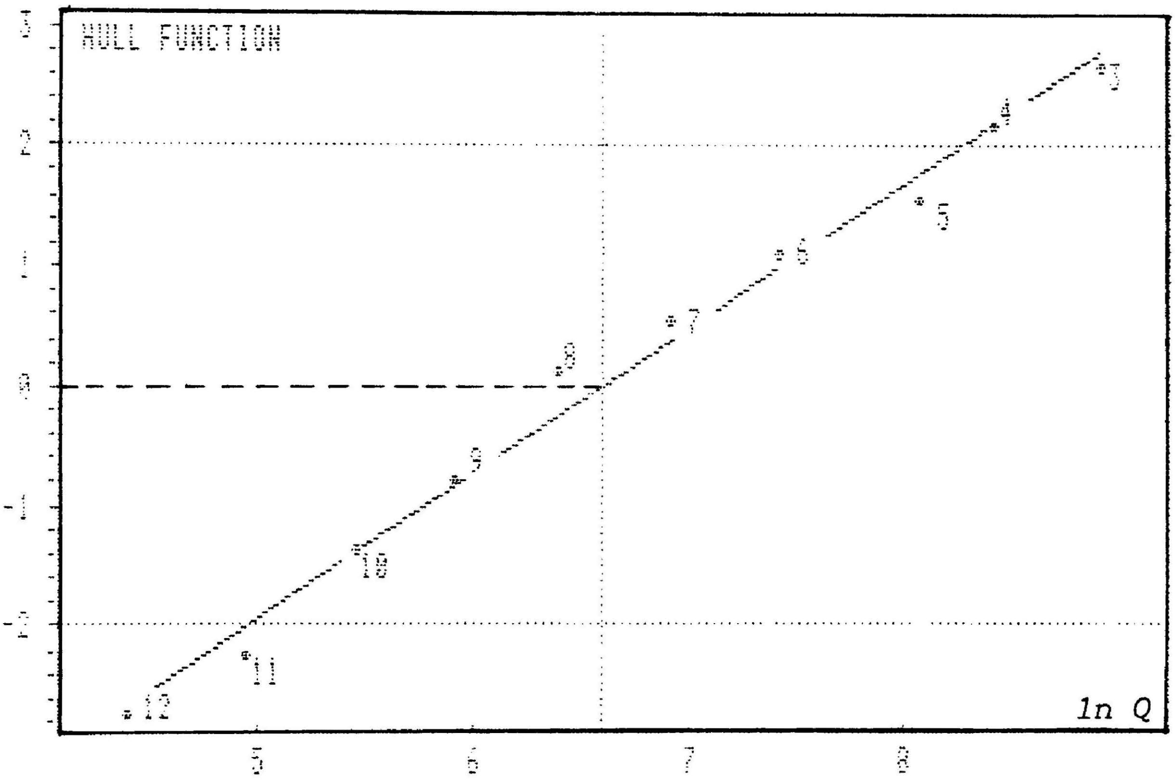

Figure 3.2: Typical Hull function plot

When quantifying, the intercept at a 50% transmission of the transmission curve gives an exposure value which is coupled to the concentration of that particular impurity element. Thus, the exposure value of an element, X, expressed as Q_X, at 50% transmission on the Hull function plot, is used as the intercept from which the concentration of element X is determined.

Natural logarithms are determined for the exposure values of element X and the internal standard, Y. A ratio of Q_x/Q_y is then calculated and used for calibration graphs to determine relative sensitivity factors (RSF's) [18]. (See pages 29 and 98).

Once relative sensitivity factors have been determined, these are stored in the software. The standard data reduction and interpretation software has been updated in this laboratory to perform the necessary calculations to determine concentrations using the relevant RSF's, exposure ratios and the internal standard concentration.

CHAPTER FOUR

QUALITATIVE SPECTRUM INTERPRETATION

4.1 U_3O_8/graphite matrix characteristics

4.1.1 General principles

Once a spectrum has been recorded on a photographic plate, each spectral line must be assigned a nominal mass. Thereafter, the lines must be related to the elements present in the sample as impurities.

The first step in assigning nominal mass values to the spectral lines is to identify the major elements. In the case of the U_3O_8/graphite matrix, majors are uranium, oxygen and carbon. A knowledge of the fingerprint spectrum of uranium is required, and is listed in Table 4.1.

Table 4.1: Mass spectrum of uranium

Charge state	Isotope	m/e	Charge state	Isotope	m/e
1+	238 235 234	238,00 235,00 234,00	4+	238 235 234	59,50 58,75 58,50
2+	238 235 234	119,00 117,50 117,00	5+	238 235 234	47,60 47,00 46,80
3+	238 235 234	79,33 78,33 78,00	6+	238 235 234	39,67 39,17 39,00

By examining the plate through a microscope, two distinct sets of spectral lines are observed in the upper half of the plate. These are distinguished as "A" and "B" in Figure 4.1. The major line of each set is due to the 238-isotope of uranium. The magnet range must be known in order to ascertain what charge state to relate to each set. In the case of Figure 4.1, the magnet range is from mass 10 to 165. Thus, from the data in Table 4.1, "A" can be assigned the mass 79,33 and "B" the mass 119,00.

At the lower end of the photoplate, a major line with dispersion due to over-saturation is noted. This line "C" is due to carbon, another major component, with mass 12. The line "D" in Figure 4.1 is due to oxygen, another major element, with mass 16.

The line marked "E" is due to the formation of the carbon dimer $^{12}C_2{}^+$ *with mass 24. The line marked "F" in Figure 4.1 is due to the formation of* $^{12}C^{16}O^+$*, the major isotopes of both carbon and oxygen, which are main components. The formation of such a species is not uncommon for a* U_3O_8*/graphite matrix.*

Once the main elements have been identified on the photoplate and nominal masses assigned to these spectral lines, these are used as markers to calibrate the rest of the data simply by filling the masses in between. It is noted that the distance between two masses at the lower end of the photoplate is larger than that obtained between two masses at the upper end. This is due to the fact that the position of a spectral line relative to any arbitrary figure is proportional to the square root of the mass-to-charge ratio, m/e [19].

A fundamental principle in the identification of spectral lines on a photoplate is to eliminate the possibility of interference

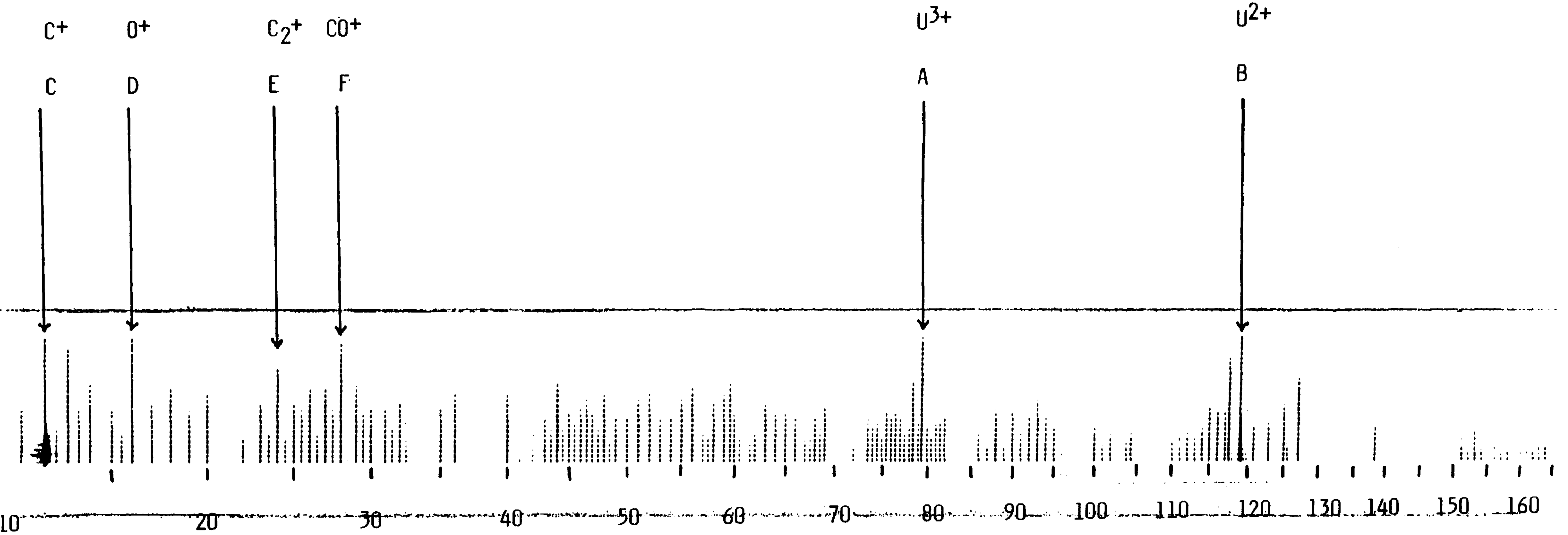

Figure 4.1: Photoplate spectrum of a U_3O_8/graphite matrix

from other elements [19]. The photoplate must be thoroughly examined so as to gain an overall impression as to which elements are present in the sample. Each element is then identified in terms of its isotopes and charge states. To positively confirm if an element is present, it must be possible to assign spectral lines on the photoplate to the elements' isotopes, as well as the various charge states. Doublets and triplets on the photoplate can be resolved on the basis of mass-defect data.

The mass defect in milli-mass units (mmu) is defined as the difference between the accurate mass and the mass number or nominal mass of an isotope. Mass-defect values for all the isotopes of the elements are relative to carbon 12 having a mass defect of zero.

Bearing in mind that the ultimate purpose is to measure the transmission of spectral lines for the quantitative determination of the elements present, it is imperative to ascertain that a spectral line is totally representative of that particular element's concentration. The importance to rule out any interference from other elements cannot be over-emphasised.

The plasma generated in the ion source is such that primarily elemental ions are formed in the U_3O_8*/graphite matrix. The formation of molecular species can largely be avoided. This simplifies matters as far as the spectrum is concerned.*

The plasma temperature must be of such a magnitude so as to prevent the formation of oxide species of the various impurity elements. When the spectrum becomes more complicated as in the case where 34 elements are present in the U_3O_8/graphite matrix, special care must be taken when assigning spectral lines with elemental names, eliminating all possibilities of interferences.

4.1.2 Selection of elements

Thirty four elements were selected from nuclear fuel specifications and are listed in Table 4.2 (see page 75). These were added to graphite powder in various ranges of concentration. The method followed for the preparation of the standards is discussed in Chapter 3 on page 26. The procedure to ascertain, firstly, whether each of these elements is present on the photoplate and, secondly, at what mass line to measure the elements present quantitatively is discussed in the following paragraphs.

4.1.3 Boron (B)

Boron		Isotopes	
Mass	1+	10	11
	2+	5	5,5
Abundance (%)		19,65	80,35
Mass defect (mmu)		+12,9	+9,3

B is positively identified at masses 10 and 11. These lines should also occur in the correct natural isotopic abundance ratios. Lines at masses 5 and 5,5 are unique to the doubly charged species of B. However, these lines are at the low-mass end of the spectrum and are not readily observed. The mass range is determined by the magnetic-field strength (H) and is selected so as to record a practical range on the photoplate.

Possible interferences at mass 10 could be the hydride species of beryllium 9 ($^{9}BeH^{+}$), the doubly charged gaseous neon 20 ($^{20}Ne^{2+}$) species or the triply charged silicon 30 ($^{30}Si^{3+}$) of small isotopic abundance (3,09%). If the concentration level of Ca is very high in the sample, the multiply charged 4+ ion of the major isotope ^{40}Ca can be detected at mass 10. However, each of these interferences appears as a doublet or triplet at mass 10, which can be resolved using the mass defect differences in milli-mass units.

Interferences at mass 11 could be the hydride species of ^{10}B, the doubly charged gaseous Ne 22 species ($^{22}Ne^{2+}$), the triply charged sulphur 33 ($^{33}S^{3+}$) of low isotopic abundance, as well as the multiply charged 4+ ion of ^{44}Ca. The mass defect of ^{11}B and these interferences are sufficient to resolve any doublets or triplets at mass 11. ^{11}B is the major isotope. The only interference of importance is the possibility that the background percentage transmission of light for the longer exposures of ^{11}B could be affected by the clouding around the longest exposures of the major component, ^{12}C, at mass 12. This is clearly manifested in Figure 4.1 at "C". To quantify B, mass 11 is the most suitable line to use.

4.1.4 Sodium (Na)

Sodium		Isotopes
Mass	1+	23
	2+	11,5
Abundance (%)		100
Mass defect (mmu)		-10,2

Na is very similar to K in that the element does not readily form multiply charged species. This is probably due to the fact that Na has only one valence electron to lose in its 3s orbital to reach the noble gas structure. Being mono-isotopic also has its disadvantages in that there is no way in which to positively identify the presence of Na other than the line at mass 23. Possible interferences could be the heterogeneous species $^{11}B^{12}C$ or the ^{46}Ca doubly charged isotope which has a low isotopic abundance (0,0037%). The most likely interference at mass 23 is the doubly charged isotope of titanium 46 ($^{46}Ti^{2+}$). The presence of this isotope of Ti can be verified by the presence of a line at mass 23,5 due to the $^{47}Ti^{2+}$ ion of similar isotopic abundance. However, this doublet can be resolved using the mass-defect value.

4.1.5 Magnesium (Mg)

Magnesium		Isotopes		
Mass	1+	24	25	26
	2+	12	12,5	13
Abundance (%)		78,84	10,08	11,09
Mass defect (mmu)		-15,0	-14,2	-17,4

The only way to positively establish whether Mg is present as an impurity is the presence of a line at mass 12,5. This line is due to the doubly charged ion of ^{25}Mg and is unique for this isotope of Mg.

Figure 4.2 represents the typical spectral lines obtained on a photoplate with Al and Mg present as impurities in a U_3O_8/graphite matrix.

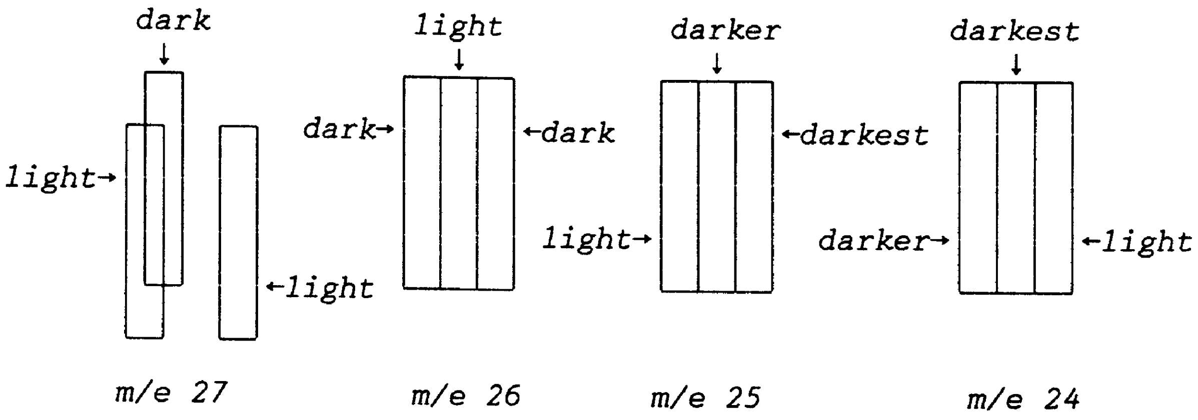

Figure 4.2: Triplet spectral lines where Mg and Al are, amongst others, present in a U_3O_8/graphite matrix (m/e 27 staggered to show overlapping).

All four spectral lines are triplets. The intensity of the blackening, which relates to the isotopic abundance of the various elemental isotopes, has also been shown. Using the reference table in Appendix B at page 180, the triplets can be resolved using the mass-defect values.

At mass 26, the light central line is due to ^{26}Mg, an isotope of small abundance. The dark left-hand line is due to the major isotope of Cr, namely $^{52}Cr^{2+}$, and the dark right-hand line could be either the hydride species of the ^{25}Mg isotope, the dimer $^{13}C_2$, or the hydrocarbon, $^{12}C_2H_2$.

At mass 25, the darker central line is due to the ^{25}Mg isotope of abundance similar to ^{26}Mg. The light left-hand line is due to the $^{50}Cr^{2+}$ isotope of small abundance (4,38%). There are three possibilities for the darkest right-hand line: it could be the hydride species of the major isotope of Mg, namely ^{24}MgH (a strong possibility), or the C dimer $^{12}C^{13}C$, or the hydrocarbon $^{12}C_2H$.

A very strong triplet appears at mass 24. There are a number of species which could give rise to this line. The most noteworthy would be the dimer of ^{12}C, the isotope of highest abundance, and the fact that C is one of the main components of the sample. The formation of C clusters is well known [20]. Other species are the doubly charged main isotope of ^{48}Ti, the main isotope of singly charged ^{24}Mg, or the doubly charged low abundance isotope of ^{48}Ca. When resolving this triplet, the central line is due to ^{24}Mg, the left-hand line due to the C dimer and the right-hand line due to $^{48}Ti^{2+}$.

All three isotopes of Mg appear as the central lines of the triplets at masses 24, 25 and 26. Because we are unable to measure the background transmission next to these lines of Mg, it is impossible to measure Mg in the singly charged state.

The close proximity of the $^{25}Mg^{2+}$ line at mass 12,5 to the line of the main component, C, at mass 12, makes the measurement of Mg unreliable because of fogging of the plate at long exposures. This affects the background transmission readings for $^{25}Mg^{2+}$ at mass 12,5.

4.1.6 Aluminium (Al)

Aluminium		Isotopes
Mass	1+	27
	2+	13,5
Abundance (%)		100
Mass defect (mmu)		-18,5

Similar to Mg, the only way to positively identify Al as an impurity in the sample is the presence of a spectral line at mass 13,5. This line is due to the doubly charged ion of the mono-isotopic ^{27}Al. In Figure 4.2 the spectral line m/e 27 represents ^{27}Al in the singly charged state. The dark central line is due to Al, the lighter left-hand line overlapping the Al line is due to a combination of $^{54}Fe^{2+}$ and $^{54}Cr^{2+}$, each isotope of low abundance. The lighter right-hand line is due to the hydride species of ^{26}Mg or the formation of the hydrocarbon $^{12}C_2H_3$. In this instance, it will be impossible to measure the central Al line because of interference from $^{54}Fe^{2+}$ and $^{54}Cr^{2+}$, as well as the fact that the microdensitometer requires a clear region on either side of a spectral line in order to measure background transmission values.

The only way to measure the mono-isotopic Al would be at its doubly charged species at mass 13,5.

4.1.7 Silicon (Si)

Silicon		Isotopes		
Mass	1+	28	29	30
	2+	14	14,5	15
Abundance (%)		92,23	4,68	3,09
Mass defect (mmu)		-23,1	-23,5	-26,2

The presence of Si is indicated by a line at mass 14,5 due to the $^{29}Si^{2+}$ isotope. This line is unique to Si only if the Ni concentration in the sample is very small. The multiply charged 4+ isotope of ^{58}Ni interferes with the $^{29}Si^{2+}$ line at mass 14,5. The difference in mass defect of these elements is so small that the two lines cannot be resolved.

At mass 28 on the photoplate a triplet is observed. Each of these lines can be resolved. The left-hand line is due to the doubly charged species of ^{56}Fe, which is the major isotope of Fe. The central line is due to the singly charged species of ^{28}Si, also the major isotope of Si. The right-hand line is somewhat lighter than the adjacent two lines. Two possible species could give rise to this line. The hydride species of the mono-isotopic ^{27}Al ion is the more probable, although the monoxide species of ^{12}C should not be discounted as C and O are both major components in the sample.

At mass 29 a weak triplet is observed. The left-hand line is much darker than the other two lines. This line is due to the doubly charged species of ^{58}Ni, which is the major isotope of Ni. The central line is the singly charged isotope of ^{29}Si, with small isotopic abundance. The right-hand line is probably due to the hydride species of the major isotope of ^{28}Si, although various other species contribute to this line, such as ^{13}CO and ^{12}CHO.

The possibility of quantitatively measuring Si in the singly charged state arises at mass 30, where a doublet is observed. These two lines can be resolved. The left-hand line is due to two species, namely the doubly charged species of ^{60}Ni, having an isotopic abundance of 26,78%, and the triply charged species $^{90}Zr^{3+}$, which is from the major isotope of Zr. The difference in mass defect of these two elements is so small that these two lines making up the left-hand line cannot be resolved. The right-hand line of the doublet is due to the singly charged species of ^{30}Si. It has been observed at times that a third line at mass 30 appears on the upper side of the ^{30}Si line, especially noticeable at very long exposures. This line could be the formation of a number of species involving C, O and H, for example $^{12}C^{18}O^{+}$, or the hydride species ^{29}Si (see reference table in Appendix B at page 180).

In order to measure the ^{30}Si line the area to the right of this line must be free of any interfering lines in order to be able to take background transmission readings. The third line does not hinder the measuring of the ^{30}Si line as it is present only at the very long exposures where the line transmission of the ^{30}Si line is in any case saturated. As the exposures get shorter, this third line fades out completely, hence enabling the measurement of the ^{30}Si line.

4.1.8 Phosphorus (P)

Phosphorus		Isotopes
Mass	1+	31
	2+	15,5
Abundance (%)		100
Mass defect (mmu)		-26,2

A line at mass 15,5 is unique to the doubly charged species of mono-isotopic ^{31}P. The singly charged species of P at mass 31 can be identified by a very dark line at long exposures. A doublet is observed, where the left-hand line is due to ^{31}P. The right-hand line, which is very low in intensity, is due to the hydride species of ^{30}Si. However, this line fades out as the exposures become shorter, as is the case at mass 30 with Si. The only possible interference with the ^{31}P line could be from the triply charged species of the mono-isotopic Nb ($^{93}Nb^{3+}$). The concentration of Nb in the sample would, however, have to be very high in order to interfere with the ^{31}P line. Before measuring the line at mass 31 for P, the presence of Nb must first be positively identified.

4.1.9 Calcium (Ca)

Calcium		Isotopes					
Mass	1+	40	42	43	44	46	48
	2+	20	21	21,5	22	23	24
Abundance (%)		96,94	0,65	0,14	2,08	0,0037	0,181
Mass defect (mmu)		-37,4	-41,4	-41,2	-44,5	-46,3	-47,6

There is no unique line for Ca on the photoplate. The only significant isotopes of Ca are at masses 40 and 44. The isotopic abundances of these isotopes are high enough, 96,94% and 2,08% respectively, to be used to identify the presence of Ca. However, interferences from other elements present in the sample hinder the measuring of these lines.

A triplet appears at mass 40. The left-hand line is the darkest in intensity and is due to the singly charged species of ^{40}Ca, the isotope with the highest abundance. This line is not unique to Ca, especially if K is also present in the sample. The line of the singly charged ^{40}K isotope overlaps with that of ^{40}Ca to the extent that the two lines cannot be resolved using the mass-defect values. The central weak line is due to the formation of two possible species. Pb and Sn are added to the standards as impurity elements originating from the reagents used to prepare the standards. The triply charged species of the ^{120}Sn isotope, which is also the isotope of highest abundance, is one of the possible species. The other is the hydride of ^{39}K, which is also the isotope of the highest abundance. The right-hand line could be due to the formation of quite a few species, of which the main possibilities are $^{28}Si^{12}C$, $^{24}Mg^{16}O$, $^{27}Al^{13}C$ and $^{12}C_2{}^{16}O$. The presence of these species is verified by the fact that they are all present in the sample as impurities and that they are the major isotopes of these elements.

At mass 44 a strong doublet is observed. The intensity of the two lines is an indication that other elements are present. The left-hand line is due to two species, namely Sr and Ca. The line of the doubly charged ^{88}Sr isotope, which has the highest abundance, overlaps with that of ^{44}Ca to the extent that the two lines cannot be resolved. The right-hand line could be due to the formation of the monoxide species of ^{28}Si. However, the more likely species is $^{12}CO_2$, a matrix-derived component of the sample. It is thus not possible to measure Ca in the singly charged state.

When considering the doubly charged state of Ca, the only isotope of importance is the major isotope, ^{40}Ca. The minor isotopes of Ca have such low abundances that they can be ignored in the doubly charged state. The line at mass 20 is due to the doubly charged species of ^{40}Ca only if the concentration of Ni in the sample is relatively low. The triply charged species of ^{60}Ni, having an isotopic abundance of 26,78%, could interfere with the line obtained from $^{40}Ca^{2+}$. This interference can be verified by the presence of a line at mass 19,33 which is due to the triply charged ^{58}Ni, the major isotope of Ni (67,18%). If there is no line present at mass 19,33 it can be assumed with certainty that there is no interference at mass 20 by $^{60}Ni^{3+}$. Ca can hence be measured using the line at mass 20.

4.1.10 Potassium (K)

Potassium		Isotopes		
Mass	1+	39	40	41
	2+	19,5	20	20,5
Abundance (%)		93,26	0,012	6,73
Mass defect (mmu)		-36,3	-36,0	-38,2

K is very similar to Na in that the element does not readily form multiply charged ions. The line obtained at mass 19,5 is very light in intensity and is unique to the doubly charged ^{39}K, the major isotope of K (93,26%). This line serves as a positive identification of K in the sample.

At mass 39 a doublet is present. The left-hand line, which is dark in intensity, is due to the singly charged species of ^{39}K, also the isotope of highest abundance. However, the presence of Sn as an impurity interferes with this line due to the triply charged species of ^{117}Sn. The two lines cannot be resolved. The right-hand line is possibly due to the C cluster $^{13}C_3$ or, if the concentration of the mono-isotopic Na and Al is very high in the sample, the formation of $^{27}Al^{12}C$ and $^{23}Na^{16}O$ species.

A poorly resolved triplet appears at mass 41. The left-hand line is due to the singly charged ^{41}K isotope with an isotopic abundance of 6,73%. The central line is the triply charged species $^{123}Sb^{3+}$ and the right-hand line is the hydride species of the major isotope of ^{40}Ca. It is thus necessary to exercise extreme care when measuring the left-hand line for K so as not to measure the central line.

4.1.11 Titanium (Ti)

Titanium		Isotopes				
Mass	1+	46	47	48	49	50
	2+	23	23,5	24	24,5	25
Abundance (%)		7,99	7,42	73,63	5,56	5,40
Mass defect (mmu)		-47,4	-48,2	-52,1	-52,1	-55,2

Ti has several isotopes which overlap with those of Ca. However, their abundances are higher, thus making Ti easier to detect. Elements which hinder the measuring of Ti in the singly charged state are Zr, Mo and Ru. The presence of these elements makes it extremely difficult to measure Ti, as their doubly charged species interfere with the lines of Ti to such an extent that they cannot be resolved. The line of ^{46}Ti has $^{92}Zr^{2+}$,

$^{46}Ca^{+}$ and $^{92}Mo^{2+}$ as interferences. The line of ^{47}Ti has $^{94}Zr^{2+}$ and $^{94}Mo^{2+}$ as its main interferences.

At mass 48 a doublet occurs. The left-hand line is that of ^{48}Ti as well as of $^{96}Mo^{2+}$, $^{48}Ca^{+}$, $^{96}Ru^{2+}$ and $^{96}Zr^{2+}$. The right-hand line is due to the possible formation of two cluster ions, namely $^{12}C_4$ and $^{24}Mg_2$. ^{49}Ti has $^{98}Mo^{2+}$, $^{98}Ru^{2+}$ and the hydride species of ^{48}Ti as interferences. Similarly, the line of ^{50}Ti has $^{50}Cr^{+}$, $^{50}V^{+}$, $^{100}Ru^{2+}$ and $^{100}Mo^{2+}$ as interferences.

The only way to positively identify the presence of Ti in the sample is to look for lines of the doubly charged species. Two isotopes of Ti, namely ^{47}Ti and ^{49}Ti, have lines at masses 23,5 and 24,5 respectively, which are unique to Ti. The only element which could possibly interfere with the line of ^{47}Ti at mass 23,5 is the multiply charged species of $^{94}Zr^{4+}$. However, the probability of such an ion forming can be tested by looking for a line at mass 22,5, due to the multiply charged species of $^{90}Zr^{4+}$, the major isotope of Zr. If no line is detected at mass 22,5, then the possibility of $^{94}Zr^{4+}$ interfering at mass 23,5 is negligible. Thus, Ti can be quantitatively measured at either of these lines.

4.1.12 Vanadium (V)

Vanadium		Isotopes	
Mass	1+	50	51
	2+	25	25,5
Abundance (%)		0,26	99,74
Mass defect (mmu)		-52,8	-56,0

V is positively identified by a line at mass 25,5 due to the doubly charged species of the major isotope of V, namely 51. The singly charged ion of V appears as a doublet at mass 51. The high intensity of the left-hand line is due to the ^{51}V isotope. The light right-hand line is that of the doubly charged ^{102}Ru^{2+} isotope. These two lines are only just resolved, thus care must be exercised when measuring the transmission of the V line so that no overlapping occurs.

4.1.13 Chromium (Cr)

Chromium		Isotopes			
Mass	1+	50	52	53	54
	2+	25	26	26,5	27
Abundance (%)		4,38	83,70	9,51	2,41
Mass defect (mmu)		-53,9	-59,5	-59,3	-61,1

Isotopes of Cr at masses 52 and 53 are used to identify and quantify Cr in the sample. The other two isotopes have interferences from Ti, V and Fe. The doubly charged species of ^{53}Cr at mass 26,5 is used to positively identify Cr as no interferences are present at this line. At mass 52 a clearly resolved doublet is present. The dark left-hand line is due to the major isotope of Cr, namely at mass 52. The light right-hand line could be the hydride species of ^{51}V or the doubly charged ion of ^{104}Ru. Various other species could also be formed in the plasma, but their influence is so small that they can be ignored (see reference table in Appendix B at page 181). When the Cr concentration is too high, the line at mass 52 is too dark to measure. The only other alternative would be to measure the ^{53}Cr line. This is not advisable due to the contribution of ^{52}CrH species.

4.1.14 Manganese (Mn) and cobalt (Co)

Manganese		Isotopes	Cobalt		Isotopes
Mass	1+	55	Mass	1+	59
	2+	27,5		2+	29,5
Abundance (%)		100	Abundance (%)		100
Mass defect (mmu)		-61,9	Mass defect (mmu)		-66,8

The mono-isotopic Mn and Co are both easily identified by their unique doubly charged ions at masses 27,5 and 29,5 respectively.

For the singly charged ^{55}Mn ion, the hydride species of ^{54}Cr and ^{54}Fe could interfere. However, the isotopic abundances of these two species are very small (2,41 and 5,90% respectively). A doublet at mass 55 is due to the doubly charged species $^{110}Cd^{2+}$, one of the numerous isotopes of Cd with a percentage abundance of only 12,46%.

Similarly, for the singly charged ^{59}Co ion, the hydride species of ^{58}Fe and ^{58}Ni could interfere. A greater possibility of interference from $^{58}NiH^{+}$ exists as the ^{58}Ni isotope is the major isotope for Ni. This species would result in a line that overlaps slightly with the Co line. Extreme care must therefore be exercised when measuring the Co line so as to not include the contribution from the $^{58}NiH^+$ species. A resolved doublet at mass 59 is the result of the doubly charged species of ^{118}Sn, one of the impurity elements added by means of the reagents used.

When the concentration level of Mn and Co is too high in the sample and the exposure pattern is such that a 50% transmission value cannot be obtained from the Hull function, the lack of other isotopes of these two elements necessitates the use of the doubly charged species to quantify Mn and Co in the sample.

4.1.15 Iron (Fe)

Iron		Isotopes			
Mass	1+	54	56	57	58
	2+	27	28	28,5	29
Abundance (%)		5,90	91,60	2,18	0,32
Mass defect (mmu)		-60,4	-65,1	-64,6	-66,7

Fe has only two isotopes of interest. The other isotopes overlap with those of Cr and Ni. The doubly charged ion of the ^{57}Fe isotope is used to positively identify the presence of Fe in the sample. A line at mass 28,5 is unique to the isotope of this element. Unreliable results are obtained when measuring this line at mass 28,5 due to $^{57}Fe^{2+}$. This occurs when the Fe concentration in the sample is not very high due to the low isotopic abundance of this isotope, namely 2,18%. It is thus preferable to measure the singly charged ions of Fe at mass 56, which is the major isotope. As in the case of $^{59}Co^+$, the line of the hydride species of Mn overlaps slightly with the line of ^{56}Fe. Thus extreme care must be exercised when measuring the transmission of the Fe line so as not to include the contribution from $^{55}MnH^+$.

A doublet at mass 56 is caused by the doubly charged species of ^{112}Cd and ^{112}Sn. When the concentration level of Fe in the sample is very high, the line at mass 56 will be oversaturated. The only alternative, as in the case of Cr, would be to measure the line at mass 57. This is, however, not advisable due to direct interference from the hydride species of ^{56}Fe namely FeH^+ at mass 57.

A doublet at mass 57 is due to the doubly charged species of ^{114}Cd and ^{114}Sn.

4.1.16 Nickel (Ni)

Nickel		Isotopes				
Mass	1+	58	60	61	62	64
	2+	29	30	30,5	31	32
Abundance (%)		67,18	26,78	1,24	3,80	1,01
Mass defect (mmu)		-64,7	-69,2	-69,0	-71,7	-72,0

A line at mass 30,5 is unique for the doubly charged ^{61}Ni isotope. However, this line can only be used when the concentration of Ni in the sample is very high, because of the very small percentage isotopic abundance, namely 1,24%. In most cases, the only method to analyse Ni would be to use the singly charged species. The isotopes at masses 58 and 64 interfere with Fe and Zn respectively. The isotopes at masses 61 and 62 are of very low abundance, making them impractical to use. Ni can be measured at mass 60 using the ^{60}Ni isotope with a relative abundance of 67,18%. As in the case of Fe and Co, the hydride species of ^{59}Co interferes with the line of ^{60}Ni. The slight overlap of the two lines can be resolved. A distinct doublet at mass 60 is due to the doubly charged species of ^{120}Sn, which is the major isotope of Sn.

4.1.17 Copper (Cu)

Copper		Isotopes	
Mass	1+	63	65
	2+	31,5	32,5
Abundance (%)		69,14	30,86
Mass defect (mmu)		-70,4	-72,2

Cu can be positively identified if lines exist at masses 31,5 and 32,5. These lines are due to the doubly charged species of the two isotopes of Cu. No interferences occur at these masses. The singly charged species of Cu at masses 63 and 65 both have the hydride species of ^{62}Ni and ^{64}Ni respectively, as interfering species. However, the isotopic abundances of these two isotopes of Ni are very small (3,80% and 1,01% respectively), thus lessening the effect their hydride species have on the Cu lines. The presence of Zn as an impurity in the sample could interfere with the line of ^{65}Cu, due to the formation of the hydride species of ^{64}Zn which is the major isotope of Zn. A doublet with slight overlapping occurs at mass 65, thus making the measuring of the Cu line unreliable. In this instance, the ^{63}Cu line should be used.

4.1.18 Zinc (Zn)

Zinc		Isotopes				
Mass	1+	64	66	67	68	70
	2+	32	33	33,5	34	35
Abundance (%)		48,89	27,77	4,12	18,59	0,638
Mass defect (mmu)		-70,9	-74,0	-72,9	-75,1	-74,7

The presence of Zn in the sample is positively identified if a line exists at mass 33,5 due to the doubly charged species of ^{67}Zn. This isotope of Zn has a low isotopic abundance (4,12%). Therefore, when the concentration level of Zn in the sample is low, no lines are observed at this mass. The singly charged species of Zn will then have to be utilised to identify the presence of Zn. The ^{64}Zn isotope cannot be used due to interference from ^{64}Ni. These two lines cannot be resolved. Another interference is the ^{63}Cu hydride whose line will overlap with that of ^{64}Zn. This leaves only the isotopes at masses 66 and 68 to measure quantitatively as the isotopes at masses 67 and 70 have too low isotopic abundances (4,12% and 0,638% respectively). The line at mass 66 has the hydride species of ^{65}Cu as interference. These two lines can be resolved using the mass-defect values. The mass-defect value for ^{65}Cu hydride is -64,4 mmu and for ^{66}Zn is -74,0 mmu. The line at mass 68 is a clearly resolved doublet. The right-hand line is due to the doubly charged species of ^{136}Ba.

4.1.19 Strontium (Sr)

Strontium		Isotopes			
Mass	1+	84	86	87	88
	2+	42	43	43,5	44
Abundance (%)		0,552	9,87	7,00	82,58
Mass defect (mmu)		-86,6	-90,7	-91,1	-94,4

The identification of Sr is quite elementary. A line at mass 43,5 is due to the doubly charged species of ^{87}Sr. However, if Rb is present in the sample, the doubly charged ^{87}Rb line interferes with that of ^{87}Sr to such an extent that the two lines cannot be resolved. If no line exists at mass 42,5 which can be uniquely assigned to the doubly charged ^{85}Rb which is the major isotope of Rb, then the line at mass 43,5 is unique to ^{87}Sr. The line at mass 88 is unique to the singly charged species of the major isotope of Sr. No interferences occur at this line.

4.1.20 Yttrium (Y)

Yttrium		Isotopes
Mass	1+	89
	2+	44,5
Abundance (%)		100
Mass defect (mmu)		-94,6

The choice of Y as the internal reference has been described on page 28. A line at mass 44,5 is unique for the doubly charged species of the mono-isotopic ^{89}Y. Similarly, a line at mass 89 is unique for the singly charged Y. The hydride species of ^{88}Sr could interfere with the line of Y at mass 89. This line of $^{88}SrH^+$ is, however, very weak in intensity and only occurs at the very long exposures.

4.1.21 Zirconium (Zr)

Zirconium		Isotopes				
Mass	1+	90	91	92	94	96
	2+	45	45,5	46	47	48
Abundance (%)		51,45	11,12	17,18	17,46	2,82
Mass defect (mmu)		-95,7	-94,8	-95,4	-93,9	-91,8

The presence of Mo and Ru in the sample makes the identification and measuring of Zr more complex as they have isotopes which overlap in mass. Furthermore, the doubly charged species of

W and Ta also interfere with the lines of these elements. The large number of isotopes, seven each for Mo and Ru and five for Zr, assists the analyst when assigning elemental names to these spectral lines.

Zr has a unique line at mass 45,5 due to the doubly charged ion of ^{91}Zr. This line serves to positively identify the presence of Zr in the sample. The singly charged ^{92}Zr and ^{94}Zr isotope lines interfere with the lines of ^{92}Mo and ^{94}Mo. Similarly, the ^{96}Zr line interferes with the lines of ^{96}Mo and ^{96}Ru. These isotope lines of Zr cannot be resolved. A line at mass 90 is, however, unique for the singly charged ion of ^{90}Zr which is the major isotope of Zr(51,45%).

A clearly resolved doublet at mass 90 is due to the doubly charged species of ^{180}W and ^{180}Ta, or the hydride species of ^{89}Y. The isotopic abundances of W and Ta are very small at these masses, thus their influence on the $^{90}Zr^{+}$ line is negligible. A line at mass 90,5 is unique for the doubly charged species of ^{181}Ta which is the major isotope of Ta. The presence of this line on the photoplate originates from the Ta present in the electrode holders.

4.1.22 Niobium (Nb)

Niobium		Isotopes
Mass	1+	93
	2+	46,5
Abundance (%)		100
Mass defect (mmu)		-94,0

The mono-isotopic Nb has a unique line at mass 46,5 due to the doubly charged ion. No other lines appear at this mass, making it unique for Nb. A doublet at mass 93 indicates the presence of W in the sample. The dark left-hand line is due to the singly charged ion of ^{93}Nb. The right-hand line is due to the doubly charged species of ^{186}W. Another possible interference for the ^{93}Nb line could be the hydride species of ^{92}Zr, ^{92}ZrH^{+}. This line cannot be resolved by the mass-defect principle. However, the isotopic abundance of ^{92}Zr is very small compared with that of the mono-isotopic Nb. Thus the ^{92}ZrH^{+} line will disappear as the exposures get shorter.

4.1.23 Molybdenum (Mo)

Molybdenum		Isotopes						
Mass	1+	92	94	95	96	97	98	100
	2+	46	47	47,5	48	48,5	49	50
Abundance (%)		15,23	9,12	15,92	16,63	9,42	24,25	9,43
Mass defect (mmu)		-93,9	-95,3	-94,3	-95,5	-94,3	-94,5	-92,4

Lines at mass 47,5 and 48,5 are unique for the doubly charged species of ^{95}Mo and ^{97}Mo. In their singly charged state these two isotopes have no interferences from other elements. As previously mentioned, ^{92}Mo, ^{94}Mo and ^{96}Mo interfere with ^{92}Zr, ^{94}Zr and ^{96}Zr; and ^{96}Mo, ^{98}Mo and ^{100}Mo interfere with ^{96}Ru, ^{98}Ru and ^{100}Ru. The isotopic abundance of ^{95}Mo is greater than that of

^{97}Mo, thus the line at mass 95 is the more suitable to measure as there are more lines present. If there is no Ru present in the sample, then the line at mass 98 due to the major isotope of Mo can be measured.

4.1.24 Ruthenium (Ru)

Ruthenium		Isotopes						
Mass	1+	96	98	99	100	101	102	104
	2+	48	49	49,5	50	50,5	51	52
Abundance (%)		5,55	1,96	12,75	12,64	17,05	31,54	18,50
Mass defect (mmu)		-92,4	-94,5	-93,9	-97,0	-95,9	-96,3	-94,5

Ru can be positively identified by the presence of lines at masses 49,5 and 50,5 due to the doubly charged ions of ^{99}Ru and ^{101}Ru respectively. No interferences occur at these masses. The isotopes of Ru at masses 96, 98 and 100 have Mo as interference in the singly charged state. These lines cannot be resolved. The same applies to the isotopes of Ru at masses 102 and 104, where the doubly charged ions of ^{204}Pb and ^{208}Pb interfere. However, these lines can be resolved using their mass-defect values. Therefore, the isotopes of Ru at masses 99, 101, 102 and 104 are unique and can be used to measure the singly charged ions of Ru.

The line at mass 102, which is from the major isotope of Ru (31,54%), gives a more reliable result because more exposure lines are present at this mass. The line due to ^{204}Pb^{2+}, which has an isotopic abundance of only 1,5%, occurs only at the very long exposures. The presence of Pd in the sample interferes with the lines of ^{102}Ru and ^{104}Ru. Thus the ^{101}Ru isotope would then be used to measure the concentration of Ru in the sample.

4.1.25 Cadmium (Cd)

Cadmium		Isotopes							
Mass	1+	106	108	110	111	112	113	114	116
	2+	53	54	55	55,5	56	56,5	57	58
Abundance (%)		1,219	0,863	12,46	12,81	24,04	12,26	28,85	7,50
Mass defect(mmu)		-94,1	-96,0	-97,0	-95,9	-97,2	-95,4	-96,44	-95,0

The difficulty of quantitatively determining Cd as an impurity at very low concentration levels is greatly compounded by the fact that Cd has no less than 8 isotopes, the highest abundance being that of ^{114}Cd at only 28,85%. Furthermore, most of the isotopes of Cd have other elements as interferences such that their lines cannot be resolved. Typically, the only isotope of Cd which can be used to positively identify the presence of Cd in the sample is the isotope at mass 111 with an abundance of only 12,81%. A line at mass 55,5 is unique for the doubly charged ion of this isotope of Cd. The line from the doubly charged ion of ^{113}Cd at mass 56,5 overlaps completely with the line of the doubly charged ion $^{113}In^{2+}$, also present in the sample. These two lines cannot be resolved using the mass-defect values.

For the singly charged species of Cd, the isotopes at masses 106, 108 and 110 have direct interference from the same isotopes of Pd if Pd is present in the sample. These lines cannot be resolved at these masses. The same applies for the isotopes at masses 112, 114 and 116, where direct interference is encountered by isotopes of Sn, one of the elements added indirectly to the standards as an impurity during the preparative stage. These lines cannot be resolved. The doubly charged ion of the mono-isotopic Th ($^{232}Th^{2+}$) produces a line at mass 116, resulting in a doublet at this mass which can be resolved. The ^{113}Cd isotope has direct interference from the ^{113}In isotope, as In is also present in the sample. Of the eight isotopes of Cd, the only isotope unique to Cd (in the singly charged state) is at mass 111, with an isotopic abundance of only 12,81%. If it can be positively shown that no Sn is present in the sample, then the lines from the ^{112}Cd and ^{114}Cd isotopes can be used to measure Cd in the singly charged state. These isotopes have isotopic abundances of 24,04% and 28,85% respectively, giving a more reliable result than that obtained from ^{111}Cd.

4.1.26 Indium (In)

Indium		Isotopes	
Mass	1+	113	115
	2+	56,5	57,5
Abundance (%)		4,24	95,76
Mass defect (mmu)		-95,7	-95,9

The presence of In in the sample can be identified by a line at mass 57,5. This line is due to the doubly charged ion of the major isotope of In, namely ^{115}In. The contribution to this line at mass 57,5 by the doubly charged ion of ^{115}Sn is negligible as the ^{115}Sn isotope has an isotopic abundance of only 0,35%. The line at mass 56,5 is due to the doubly charged ion of ^{113}Cd which interferes directly with the line of the doubly charged ion of ^{113}In. These two lines cannot be resolved. The isotopic abundance of ^{113}In is in any case too small for the doubly charged ion of this isotope of In to be detected at mass 56,5.

The only singly charged isotope of In which can be used to quantify In in the sample is ^{115}In. The line at this mass is dark in intensity, coinciding with the isotopic abundance of this isotope of In, namely 95,75%. However, the longest exposure lines have interference from the ^{115}Sn isotope, with an isotopic abundance of only 0,35%. The 50% transmission intercept obtained for this line at mass 115 is unique for ^{115}In and can be used to quantify In in the sample.

4.1.27 Antimony (Sb)

Antimony		Isotopes	
Mass	1+	121	123
	2+	60,5	61,5
Abundance (%)		57,25	42,75
Mass defect (mmu)		-96,3	-95,9

Sb has only two isotopes, namely at masses 121 and 123, with abundances that are roughly the same (57,25 and 42,75% respectively). This facilitates the detection of Sb as an impurity in the sample. The doubly charged ions of both isotopes of Sb yield lines at masses 60,5 and 61,5 which are unique for Sb. If Te is present in the sample, the contribution from the doubly charged ion of ^{123}Te at mass 61,5, with an isotopic abundance of only 0,88%, can be considered negligible.

In the singly charged state, it is preferable to use the line at mass 123 instead of the line at mass 121, both due to the isotopes of singly charged Sb, because of fogging caused by the major isotope of uranium, one of the main components in the sample. The doubly charged ion of ^{238}U yields a very intense line at mass 119, causing the fogging. This is similar to what happens to $^{11}B^{+}$ and $^{25}Mg^{2+}$, caused by the fogging of ^{12}C. However, when Te is present and can be positively identified in the sample, there is no alternative but to measure the line at mass 121 in order to quantify Sb. The result so obtained would be more unreliable than that obtained if the line at mass 123 is measured.

4.1.28 Barium (Ba)

Barium		Isotopes						
Mass	1+	130	132	134	135	136	137	138
	2+	65	66	67	67,5	68	68,5	69
Abundance (%)		0,108	0,119	2,44	6,58	7,87	11,41	71,50
Mass defect (mmu)		-93,8	-94,9	-95,7	-94,4	-95,6	-94,4	-95,0

Lines observed at masses 67,5 and 68,5 are unique for the doubly charged ions of ^{135}Ba and ^{137}Ba, respectively. No interferences occur at these masses. It is preferable to measure the line at mass 68,5 instead of at 67,5, as ^{137}Ba has a higher isotopic abundance than ^{135}Ba, providing more exposure lines on the photoplate. The line at mass 138 is used to quantify Ba in the sample. This line is due to the singly charged ion of the major isotope of Ba at mass 138, with an isotopic abundance of 71,5%. If La and Ce were present in the sample, they would interfere with the line of ^{138}Ba. However, these two isotopes of La and Ce have very small isotopic abundances of only 0,089% and 0,258%, respectively, and their influence can be ignored. They would probably only interfere at the longest exposure lines, which would then in any case be saturated for Ba.

4.1.29 Tungsten (W), bismuth (Bi) and thorium (Th)

For the next three elements, namely W, Bi and Th, the only way to positively identify and quantify their presence in the sample is to consider only their doubly charged species. This restriction is imposed because the mass range of the magnet has been chosen so as to only go up to mass 165 for the purpose of this investigation.

Tungsten		Isotopes				
Mass	1+	180	182	183	184	186
	2+	90	91	91,5	92	93
Abundance (%)		0,137	26,22	14,32	30,66	28,66
Mass defect (mmu)		-53,0	-51,7	-49,7	-49,0	-45,7

A line at mass 91,5 is unique for the doubly charged ion of ^{183}W. The isotopic abundance of this isotope is only 14,32%, making it unfavourable to use at low concentration levels in the sample. However, the other isotopes of W, at masses 182, 184 and 186, with isotopic abundances of 26,22%, 30,66% and 28,66% respectively, give clearly resolved doublets at masses 91, 92 and 93. These doublets can be resolved using their mass-defect values. As discussed earlier, the doublet at mass 91 would be ^{91}Zr, that at mass 92 would be a combination of both ^{92}Zr and ^{92}Mo and that at mass 93 would be the mono-isotopic Nb. By carefully setting up the microdensitometer, each line of the doublet can be measured simultaneously, without any uncertainty of the result so obtained.

Bismuth		*Isotopes*
Mass	*1+*	*209*
	2+	*104,5*
Abundance (%)		*100*
Mass defect (mmu)		*-19,6*

The presence of Bi in the sample can be positively identified if a line appears at mass 104,5. This line is due to the doubly charged ion of the mono-isotopic ^{209}Bi and is unique for Bi.

Thorium		*Isotopes*
Mass	*1+*	*232*
	2+	*116*
Abundance (%)		*100*
Mass defect (mmu)		*+38,2*

A clearly resolved doublet at mass 116 indicates the presence of Th in the sample. The left-hand line is due to a combination of both the singly charged ion for ^{116}Cd and the singly charged ion of ^{116}Sn. The darker right-hand line is due to the doubly charged ion of the mono-isotopic ^{232}Th. This line is unique and can be measured to quantify Th.

4.1.30 Samarium (Sm)

Samarium		Isotopes						
Mass	1+	144	147	148	149	150	152	154
	2+	72	73,5	74	74,5	75	76	77
Abundance (%)		3,03	14,92	11,21	13,81	7,39	26,84	22,97
Mass defect (mmu)		-88,4	-85,4	-85,4	-83,1	-83,0	-80,5	-78,0

Lines at masses 73,5 and 74,5 are unique for the doubly charged Sm isotopes 147 and 149 respectively. No interference from other elements occurs at these masses. In the singly charged state, the only isotopes unique for Sm are at masses 147 and 149. The isotopes with masses 144, 148 and 150, of relatively low abundance, can have Nd as interference. Similarly, the isotopes with masses 152 and 154, both major isotopes of Sm, have Gd as interference. Of the remaining two isotopes unique for Sm, the ^{147}Sm isotope is used to measure quantitatively because of the higher abundance, namely 14,92%.

4.1.31 Europium (Eu)

Europium		Isotopes	
Mass	1+	151	153
	2+	75,5	76,5
Abundance (%)		47,79	52,21
Mass defect (mmu)		-80,4	-79,1

Both the isotopes of Eu are unique for this element. No interferences from other elements occur. The presence of Eu in the sample is positively identified by the presence of lines at masses 75,5 and 76,5. These two lines are due to the doubly charged ions of the two isotopes of Eu, namely ^{151}Eu and ^{153}Eu, respectively. For Eu in the singly charged state, either of the lines at masses 151 and 153 can be used to quantify Eu as the abundances of these two isotopes are very similar.

4.1.32 Gadolinium (Gd)

Gadolinium		Isotopes						
Mass	1+	152	154	155	156	157	158	160
	2+	76	77	77,5	78	78,5	79	80
Abundance (%)		0,20	2,16	14,87	20,56	15,70	24,77	21,79
Mass defect (mmu)		-80,5	-79,3	-77,4	-77,9	-76,1	-75,9	-72,9

Gd is very similar to Sm in that it also has only two isotopes which are unique to it, namely ^{155}Gd and ^{157}Gd. The doubly charged ions of these two isotopes of Gd give lines at masses 77,5 and 78,5, respectively, which are used to identify the presence of Gd in the sample. No interference from other elements occurs at these masses.

When measuring the doubly charged state of Gd, it is preferable to use the line at mass 77,5, because the line at 78,5 is obscured by the line of $^{235}U^{3+}$ at mass 78,33 (U being one of the main components in the sample.) In the singly charged state, ^{152}Gd and ^{154}Gd, both of low abundance, have Sm as interference. The three major isotopes of Gd, namely ^{156}Gd, ^{158}Gd and ^{160}Gd, have Dy as interference. The isotope suitable to quantify Gd in the singly charged state is the ^{157}Gd which has a higher abundance than ^{155}Gd.

4.1.33 Dysprosium (Dy)

Dysprosium		Isotopes						
Mass	1+	156	158	160	161	162	163	164
	2+	78	79	80	80,5	82	81,5	82
Abundance (%)		0,058	0,098	2,33	18,87	25,46	24,93	28,25
Mass defect (mmu)		-76,2	-76,0	-75,2	-74,3	-73,5	-71,6	-71,2

The doubly charged ions of Dy with masses 161 and 163 give lines at masses 80,5 and 81,5 which are unique for Dy. In the singly charged state the first three isotopes of Dy (namely at masses

156, 158 and 160), all with very low isotopic abundance, have Gd as interference. The remaining four isotopes of Dy, with abundances ranging from 18,87 % to 28,25%, can be used to quantify Dy in the singly charged state. However, the presence of Er in the sample would interfere at masses 162 and 164. ^{163}Dy would then be used as it is unique for Dy and has a higher abundance than ^{161}Dy.

4.1.34 Selection of isotopes and charge states

The choice of isotopes used to identify and quantify each of the 34 elements present in the U_3O_8/graphite matrix is summarised in Table 4.2.

Table 4.2: Isotopes and charge states used to quantify impurity elements in a U_3O_8/graphite matrix

Element	Charge state	m/e	Isotope	Abundance (%)
B	1+	11	11	80,35
Na	1+	23	23	100
Mg	2+	12,5	25	10,08
Al	2+	13,5	27	100
Si	1+ 2+	30 14,5	30 29	3,09 4,68
P	1+ 2+	31 15,5	31 31	100 100
Ca	2+	20	40	96,94
K	1+ 2+	41 19,5	41 39	6,73 93,26

Table 4.2: Continued

Element	Charge state	m/e	Isotope	Abundance (%)
Ti	1+	48	48	73,63
	2+	23,5	47	7,42
V	1+	51	51	99,74
	2+	25,5	51	99,74
Cr	1+	52	52	83,70
	2+	26,5	53	9,51
Mn	1+	55	55	100
	2+	27,5	55	100
Fe	1+	56	56	91,60
	2+	28,5	57	2,18
Co	1+	59	59	100
	2+	29,5	59	100
Ni	1+	60	60	26,78
Cu	1+	63	63	69,16
	2+	31,5	63	69,14
Zn	1+	66	66	27,77
Sr	1+	88	88	82,58
	2+	43,5	87	7,00
Zr	1+	90	90	51,45
	2+	45,5	91	11,12
Y	1+	89	89	100
	2+	44,5	89	100
Nb	1+	93	93	100
	2+	46,5	93	100
Mo	1+	95	95	15,92
	2+	47,5	95	15,92
Ru	1+	102	102	31,54
	2+	50,5	101	17,05
Cd	1+	111	111	12,81

Table 4.2: Continued

Element	Charge state	m/e	Isotope	Abundance (%)
In	1+ 2+	115 57,5	115 115	95,76 95,76
Sb	1+ 2+	123 61,5	123 123	42,75 42,75
Ba	1+ 2+	138 68,5	138 137	71,50 11,41
Sm	1+ 2+	147 73,5	147 147	14,92 14,92
Eu	1+ 2+	153 76,5	153 153	52,21 52,21
Gd	1+ 2+	157 78,5	157 157	15,70 15,70
Dy	1+ 2+	163 81,5	163 163	24,93 24,93
W	2+	93	186	26,66
Bi	2+	104,5	209	100
Th	2+	116	232	100

4.2 UF_4/graphite matrix characteristics

4.2.1 General principles

The qualitative interpretation of a UF_4/graphite matrix spectrum is far more complex than that of a U_3O_8/graphite matrix. The over-abundance of fluoride ions generated in the plasma from UF_4 leads to fluorination and recombination of elemental ions present in the sample as impurities. When 0,004 moles of UF_4 is used to prepare electrodes with graphite, this mass of UF_4 yields a concentration of fluorine of 320 000 µgF/gU, compared with the total concentration of impurities in the UF_4 sample of perhaps up to 1 000 µg/gU. Because fluorine is so extremely reactive with other elements and, as indicated above, in total abundance, the chances of fluorination are greatly enhanced. This phenomenon complicates the interpretation of the mass spectrum of a UF_4/graphite matrix.

The procedures followed for assigning nominal mass values to the spectral lines on a photoplate exposed to a UF_4/graphite matrix are very similar to those for a U_3O_8/graphite matrix. The major elements must first be identified. The fingerprint spectrum of uranium is given in Table 4.1 on page 38. By examining the photoplate through a microscope, several major lines are observed over the entire length of the photoplate. These lines are distinguished by A, B, C, D, E, F, G and H in Figure 4.3. The two distinct lines in the upper half of the photoplate, "A" and "B", are due to the major isotope of U, i.e. ^{238}U. The magnet range in Figure 4.3 is from mass 10 to mass 130. Thus, from the data given in Table 4.1, "A" can be assigned the mass 119 and "B" the mass 79,33, which corresponds with the ions $^{238}U^{2+}$ and $^{238}U^{3+}$ respectively.

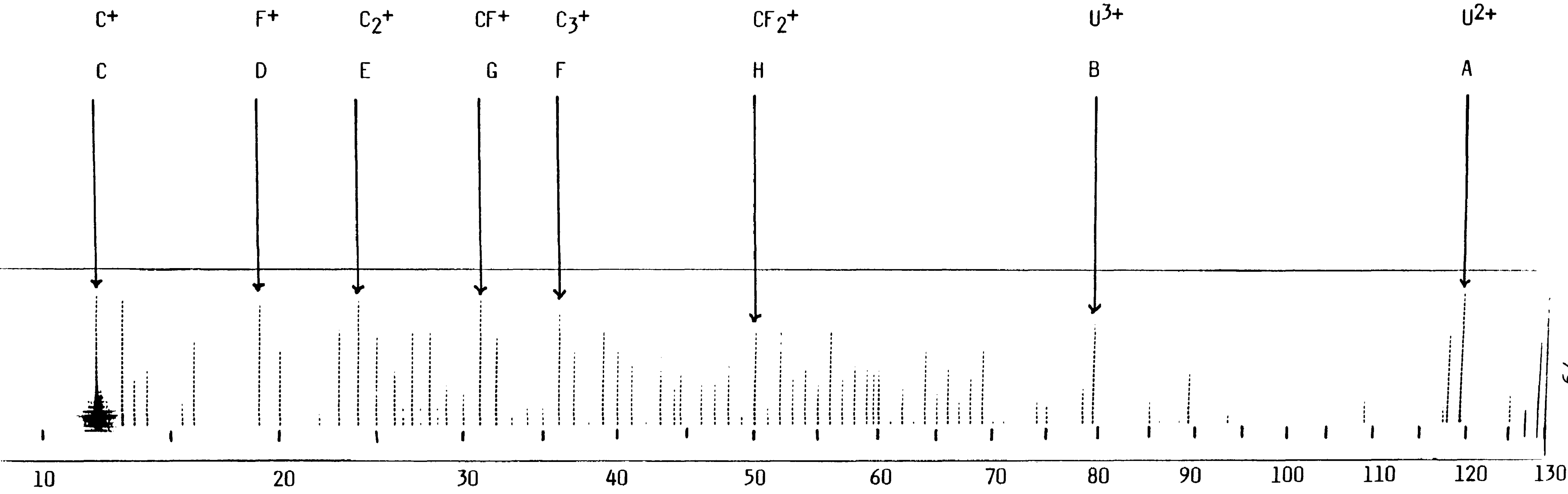

Figure 4.3: Photoplate spectrum of a UF_4/graphite matrix

At the lower end of the photoplate, the strong line with dispersion, marked "C", can be assigned the mass 12. This is due to another major component, C. Similarly, the line marked "D" can be assigned the nominal mass of 19, due to a main component, F.

The lines marked "E" and "F" in Figure 4.3 are due to the clusters C_2^+ and C_3^+ respectively, at masses 24 and 36. The formation of carbon clusters is well known [20].

The lines marked "G" and "H" are due to the formation of fluorinated carbon species, CF^+ and CF_2^+, with nominal masses 31 and 50, respectively. The formation of such species is not uncommon for a UF_4/graphite matrix. By using the above markers on the photoplate, the rest of the lines can be assigned nominal mass values to calibrate the rest of the photoplate data.

The positive identification of an element as an impurity in a UF_4/graphite matrix is not always possible. A vast number of fluorinated species of other elements could interfere with the lines of the element under investigation. This limits the use of singly charged species to quantify an element, unless a doublet or triplet can be satisfactorily resolved using mass-defect values.

Each element (X) present in the UF_4 sample, with all its isotopes, forms fluorinated species of up to $XF_{(n-1)}$, where n is the number of fluorine atoms present in that element's stable state, e.g. where X=P, we get PF_5 and where X=S, we get SF_6 [21, 22]. When too many elements are present in the UF_4, the qualitative interpretation of the spectrum obtained becomes too complicated as the interferences of fluorinated species do not permit the positive identification of a single line which is totally representative of a particular element. This is in stark contrast *to the analysis of a U_3O_8/graphite matrix discussed in Section 4.1, where 34 elements of interest could be positively identified and measured. This was possible because of the formation of primarily elemental ions in the plasma, hence avoiding the great number of possible molecular ion interferences.*

4.2.2 Selection of elements

Seven elements were identified in the study of reactions in the uranium fuel production process. The UF_4-material had to be analysed qualitatively and quantitatively in the solid state, without prior chemical treatment. The spark-source mass spectrometer made a significant contribution to these studies.

The seven elements listed in Table 4.3 (see page 97) were added to graphite powder at five concentration levels. The method followed for the preparation of these standards is discussed in Chapter 3 on page 26.

4.2.3 Aluminium (Al)

Aluminium		Isotopes
Mass	1+	27
	2+	13,5
Abundance (%)		100
Fluorinated species	AlF^+	46
	AlF_2^+	65
	AlF_3^+	84

A line at mass 13,5 is unique for the doubly charged ion of the mono-isotopic ^{27}Al and is used to measure Al quantitatively. The singly charged ion at mass 27 appears as a triplet which can be resolved using the mass-defect values. Possible interferences at mass 27 are the doubly charged ions of ^{54}Cr and ^{54}Fe. The presence of these two elements in the sample can be verified by lines at masses 26,5 and 28,5 due to the doubly charged state of ^{53}Cr and ^{57}Fe respectively. Another possible interference could be the doubly charged ion of fluorinated chlorine (^{35}Cl), namely $^{35}ClF^{2+}$. By using the mass-defect value, it can be shown that the central line at mass 27 is due to the singly charged ion of Al, which cannot be used for quantification.

The formation of AlF^{+} is confirmed by a single line at mass 46. However, quite a few interferences could contribute to this line. The mono-isotopic ions of ^{46}Ca and ^{46}Ti could interfere, as well as the fluorinated species $^{54}FeF_2^{2+}$ and $^{35}ClF_3^{2+}$.

A doublet is observed at mass 65. Possible interferences at this mass, resulting in a doublet, could be from the $^{65}Cu^{+}$ ion, which must first be positively identified by the presence of lines at masses 31,5 and 32,5, due to the doubly charged ions of the two isotopes ^{63}Cu and ^{65}Cu, respectively. Other interferences could be the fluorinated species of Al, namely $^{27}AlF_2^{+}$, and of Ca, namely $^{46}CaF^{+}$.

A light single line at mass 84 could be due to the formation of $^{27}AlF_3^{+}$. This line could also be from the fluorinated species of ^{65}Cu, namely CuF^{+}.

4.2.4 Phosphorus (P)

Phosphorus		Isotopes
Mass	1+	31
	2+	15,5
Abundance (%)		100
Fluorinated species	PF^+	50
	PF_2^+	69
	PF_3^+	88
	PF_4^+	107
	PF_5^+	126

The table below illustrates the fluorination of ^{12}C, which helps to enlighten the interferences of these two elements.

Carbon		Isotopes
Mass	1+	12
Abundance (%)		98,89
Fluorinated species	CF^+	31
	CF_2^+	50
	CF_3^+	69
	CF_4^+	88

The doubly charged ion of the mono-isotopic ^{31}P yields a doublet at mass 15,5. This doublet can be resolved using the mass-defect values. The darker left-hand line is due to P^{2+} and the light right-hand line due to the doubly charged ion of $^{12}CF^{2+}$. The only line of P which can be used to measure P in the sample is this left-hand line at mass 15,5.

The singly charged ion of P at mass 31 appears as a very dark unresolved doublet. The interference is due to the fluorinated species of C, namely $^{12}CF^{+}$. Another species which could interfere at this mass is the doubly charged ion of ^{62}Ni, which can be positively identified as being present in the sample if a line appears at mass 30,5, due to $^{61}Ni^{2+}$.

For the fluorinated species of P, lines are observed up to the formation of PF_4^+. No line is observed at mass 126 due to PF_5^+.

A doublet appears at mass 50, one line due to PF^+ and the other due to CF_2^+. Similarly, a doublet appears at mass 69, one of the lines due to PF_2^+ and the other due to CF_3^+. At masses 88 and 107, single lines are present. The line at mass 88 is due to the presence of PF_3^+ and the line at mass 107 is due to PF_4^+. No interference from other fluorinated species occurs at these two lines, although the fluorinated carbon species, CF_4^+, with a mass of 88, does interfere with the PF_3^+ ion.

4.2.5 Calcium (Ca)

Calcium		Isotopes					
Mass	1+	40	42	43	44	46	48
	2+	20	21	21,5	22	23	24
Abundance (%)		96,94	0,65	0,1	2,08	0,0037	0,181
Fluorinated species	CaF^+	59	61	62	63	65	67
	CaF_2^+	78	80	81	82	84	86

The doubly charged ion of the major isotope of Ca, namely $^{40}Ca^{2+}$, appears as a doublet at mass 20. This doublet can be resolved using the mass-defect values. The strong right-hand line is due to the formation of HF^+, a species which occurs readily in a UF_4/graphite matrix. The left-hand line, due to $^{40}Ca^{2+}$, is used to measure Ca quantitatively.

The ^{42}Ca isotope is also used to measure Ca quantitatively. The result obtained is used as a guide to check whether the correct line of the doublet was selected at mass 20, as the two measurements should give the same result. It is not always possible to do this as the doubly charged ion of ^{42}Ca is only observed when the Ca concentration in the sample is fairly high. The isotopic abundance of ^{42}Ca is only 0,65%, yielding a very faint line at mass 21. However, this line is single and unique for ^{42}Ca. Lines at masses 21,5 and 22 can also be used to identify the presence of Ca in the sample. The line at mass 21,5 is too light to measure (abundance 0,14%) and the line at mass 22 has interferences from $^{25}MgF^{2+}$ and possibly $^{12}C^{13}CF^{2+}$, (C_2F^{2+}), which cannot be resolved.

There are too many interferences to measure Ca in the singly charged state. For ^{40}Ca there is interference from ^{40}K, the presence of which is identified by a line at mass 19,5, due to the ^{39}K doubly charged ion. For ^{42}Ca, interference is in the form of $^{65}CuF^{2+}$ and NaF^+. The presence of Na in the sample is confirmed by a strong line at mass 23. At mass 43, ^{43}Ca has interference from $^{24}MgF^+$ and $^{12}C_2F^+$. The formation of $^{24}MgF^+$ is confirmed by the presence of a line at mass 12,5 due to the doubly charged ion of ^{25}Mg. Similarly, for ^{44}Ca, interferences are $^{25}MgF^+$ and $^{12}C^{13}CF^+$.

The isotopic abundance of ^{46}Ca is so small that this isotope can be ignored, although possible interferences are $^{27}AlF^+$ and $^{46}Ti^+$, the presence of which is confirmed by lines at masses 23,5 and 24,5 due to the doubly charged ions of ^{47}Ti and ^{49}Ti, respectively.

Furthermore, the interpretation of the Ca spectrum is made more complex by the fluorination of Ca to form CaF^+ species with all the isotopes. The interferences on the lines of the CaF^+ species is such that no line can be uniquely assigned. This is detailed below:

- The line at mass 59 is a doublet due to $^{59}Co^+$ and $^{40}CaF^+$;
- that at mass 61 is also a doublet due to $^{61}Ni^+$ and $^{42}CaF^+$;
- that at mass 62 a weak doublet due to $^{62}Ni^+$ and $^{43}CaF^+$; and
- that at mass 63 a doublet due to $^{63}Cu^+$ and $^{44}CaF^+$.

The line at mass 65 could be due to a combination of $^{65}Cu^+$, $^{46}CaF^+$, $^{46}TiF^+$ and $^{27}AlF_2^+$. Similarly, the line at mass 67 could be due to a combination of $^{67}Zn^+$, $^{48}CaF^+$, $^{48}TiF^+$ and $^{29}SiF_2^+$.

No line is observed at mass 78, which would indicate the formation of $^{40}CaF_2^+$.

4.2.6 Silicon (Si)

Silicon		Isotopes		
Mass	1+	28	29	30
	2+	14	14,5	15
Abundance (%)		92,23	4,68	3,09
Fluorinated species	SiF^+	47	48	49
	SiF_2^+	66	67	68
	SiF_3^+	85	86	87
	SiF_4^+	104	105	106

The presence of Si in the sample can be positively identified by a single line at mass 14,5 due to the doubly charged ion of ^{29}Si. This line cannot be measured to quantify Si, as it is very weak in intensity because of the ^{29}Si abundance of only 4,68%.

In the singly charged state the lines of the various Si isotopes have interferences to contend with. At mass 28 there are four overlapping lines which cannot be resolved using mass-defect values.

Apart from the line for ^{28}Si, other interferences are $^{56}Fe^{2+}$, $^{37}ClF^{2+}$ and $^{65}CuF^{3+}$. From the intensity of the central line it would appear as if this line is due to ^{28}Si, the major Si isotope. At mass 29 an unresolved triplet is observed, made up of the interferences of $^{58}Fe^{2+}$, $^{58}Ni^{2+}$ and possibly $^{39}KF^{2+}$, with the line of ^{29}Si. The presence of K in the sample can be verified by a line at mass 19,5 due to the doubly charged ion of ^{39}K.

A resolved triplet is found at mass 30. The left-hand line is due to the doubly charged ion of ^{60}Ni. The central line is due to ^{30}Si and the right-hand line is due to either $^{12}C_5{}^{2+}$ or $^{41}KF^{2+}$. The formation of $^{41}KF^{+}$ is verified by the presence of a strong doublet at mass 60 due to $^{60}Ni^{+}$ and $^{41}KF^{+}$. The right-hand line of the triplet at mass 30 is weak in intensity, thus it does not affect the measuring of the ^{30}Si central line. Only the saturated exposures of ^{30}Si have any interference from this weak right-hand line. This is the only Si line which can be measured to quantify Si.

Silicon forms several fluorinated species. For the formation of SiF^{+}species the following lines are obtained:

- *A doublet at mass 47 due to $^{28}SiF^{+}$ and $^{47}Ti^{+}$;*
- *a doublet at mass 48 due to several possible species, e.g. $^{29}SiF^{+}$,$^{12}C_4{}^{+}$, $^{48}Ti^{+}$, $^{48}Ca^{+}$; and*
- *a doublet at mass 49 due to $^{30}SiF^{+}$, $^{49}Ti^{+}$ and $^{12}C_3{}^{13}C^{+}$.*

For the formation of $SiF_2{}^{+}$ species, the following lines are obtained which can be resolved using mass-defect values:

- *A triplet at mass 66, where the left-hand line is due to $^{66}Zn^{+}$;*
- *a weak central line due to $^{47}TiF^{+}$; and*
- *a strong right-hand line due to $^{28}SiF_2{}^{+}$.*

At mass 67 a triplet is present, where

- the weak left-hand line is due to $^{67}Zn^+$ with small abundance;
- the strong central line is that of $^{48}TiF^+$, the major isotope of Ti combined with $^{48}CaF^+$; and
- the weak right-hand line is due to $^{29}SiF_2^+$.

Similarly,at mass 68, a weak triplet is observed, where

- the stronger left-hand line is due to $^{68}Zn^+$;
- the weak central line is due to $^{49}TiF^+$; and
- the weak right-hand line is due to $^{30}SiF_2^+$.

For the formation of SiF_3^+ species, the only line obtained is that of the major isotope of Si, which gives a single line at mass 85 due to the formation of $^{28}SiF_3^+$. No line is observed at mass 104 to confirm the presence of SiF_4^+ species.

4.2.7 Sulphur (S)

Sulphur		Isotopes			
Mass	1+	32	33	34	36
	2+	16	16,5	17	18
Abundance (%)		95,0	0,76	4,22	0,01
Fluorinated species	SF^+	51	52	53	55
	SF_2^+	70	71	72	74
	SF_3^+	89	90	91	93
	SF_4^+	108	109	110	112
	SF_5^+	127	128	129	131
	SF_6^+	146	147	148	150

For the formation of fluorinated S species, the table below illustrates the fluorinated species of ^{13}C, and the interferences of these two elements.

Carbon		Isotopes
Mass	1+	13
Abundance (%)		1,10
Fluorinated species	CF^{+}	32
	CF_2^{+}	51
	CF_3^{+}	70
	CF_4^{+}	89

The doubly charged ion of the ^{33}S isotope gives a line at mass 16,5. However, no line is observed at this mass because the isotopic abundance of the ^{33}S is only 0,76%. This means that only the singly charged state of S can be used to quantify S in the sample.

At mass 32 there is a doublet which can be resolved. The main interference at this mass is from the major isotope of Zn, namely $^{64}Zn^{2+}$. Other possible interferences are $^{13}CF^{+}$ and $^{64}Ni^{2+}$. The right-hand line of this doublet is due to $^{32}S^{+}$, which is used to measure S.

The ^{33}S and ^{36}S isotopes both have very small abundances, with the result that their lines at masses 33 and 36 are so faint that they cannot be used. This is apart from the fact that ^{33}S also has $^{66}Zn^{2+}$ as interference and ^{36}S has the cluster $^{12}C_3^{+}$ as interference.

A very weak doublet is obtained at mass 34 due to $^{34}S^+$ and $^{68}Zn^{2+}$. These two lines overlap to such an extent that they cannot be resolved on the basis of the mass-defect values.

Only the ^{32}S and ^{34}S isotopes are used to illustrate the fluorination of S to form $SF_n{}^+$ species, where n=1 and 2. For SF^+ a doublet is obtained at mass 51 due to $^{32}SF^+$, $^{13}CF_2{}^+$ and $^{51}V^+$, the presence of which in the sample can be identified by a line at mass 25,5, which is unique for $^{51}V^{2+}$. Similarly, a doublet is obtained at mass 53 due to $^{34}SF^+$ and $^{53}Cr^+$. For the formation of $SF_2{}^+$ species, a doublet at mass 70 is due to $^{32}SF_2{}^+$, $^{13}CF_3{}^+$ and the fluorinated species of V, namely $^{51}VF^+$, as interferences. A doublet at mass 72 originates from $^{34}SF_2{}^+$ and $^{53}CrF^+$. In the same way that the fluorinated species of ^{12}C interfered with the fluorinated species of P, the fluorinated species of ^{13}C interfere with the fluorinated species of S up to the formation of $^{13}CF_3{}^+$ species.

For the formation of further $SF_n{}^+$ species where n = 3, 4 and 5, only the major isotope, ^{32}S, will be considered. At mass 89 a clearly resolved doublet is obtained. The dark line is that of the internal standard, the mono-isotopic ^{89}Y, and the very weak line is that of $^{32}SF_3{}^+$ which does not interfere with the 50% transmission intercept obtained for ^{89}Y, except at the longest exposures. A line at mass 108 is due to the formation of $^{32}SF_4{}^+$ and/or the formation of YF^+. Similarly, a line at mass 127 is a combination of $^{32}SF_5{}^+$, $^{89}YF_2{}^+$ and $^{235}UF^{2+}$. No line is obtained at mass 146 to confirm the presence of $SF_6{}^+$ species.

4.2.8 Chlorine (Cl)

Chlorine		Isotopes	
Mass	1+	35	37
	2+	17,5	18,5
Abundance (%)		75,72	24,28
Fluorinated species	ClF^+	54	56
	ClF_2^+	73	75
	ClF_3^+	92	94
	ClF_4^+	111	113
	ClF_5^+	130	132

No lines are readily observed at masses 17,5 and 18,5, which would be due to the doubly charged species of ^{35}Cl and ^{37}Cl respectively. The lines for Cl in the singly charged state are used to identify the presence of Cl in the sample, as well as to quantify Cl.

At mass 35 a weakly resolved doublet is observed. The strong left-hand line is due to ^{35}Cl, the major isotope of Cl. The faint right-hand line could be $^{70}Zn^{2+}$, or the species $^{16}OF^+$. These interferences do not affect the measuring of the ^{35}Cl line as they only occur at the very long exposures.

At mass 37 there is a clearly resolved doublet. The weaker left-hand line is due to $^{37}Cl^+$ and the strong right-hand line is due to the formation of the cluster $^{12}C_2{}^{13}C$ (C_3).

Both lines of Cl are measured, the ^{37}Cl line being used as a check for the ^{35}Cl line. The results obtained from each line should ideally be the same.

The fluorination of Cl cannot be positively verified. This is a result of the numerous interferences of fluorinated species of Cr and Fe. The formation of ClF^+ species would give rise to lines at masses 54 and 56. Interferences at mass 54 are $^{54}Cr^+$ and $^{54}Fe^+$, both elements having low abundance. At mass 56 the major isotope of ^{56}Fe results in a doublet with the $^{37}ClF^+$ species.

The formation of ClF_2^+ species would result in lines at masses 73 and 75. The single line at mass 73 could be due to $^{35}ClF_2^+$, $^{54}FeF^+$ or $^{54}CrF^+$. The doublet at mass 75 could be as a result of the formation of $^{37}ClF_2^+$ and the fluorinated species of the major isotope of Fe, namely $^{56}FeF^+$.

Similarly, the formation of ClF_3^+ species would result in faint lines at masses 92 and 94. Apart from $^{35}ClF_3^+$, the line at mass 92 could also be due to $^{54}FeF_2^+$ and $^{54}CrF_2^+$. The line at mass 94 could be the result of a combination of $^{37}ClF_2^+$ and $^{56}FeF_2^+$.

The formation of ClF_4^+ species cannot be positively verified as no lines are observed at masses 111 and 113. No lines appear at masses 130 and 132 to confirm the presence of ClF_5^+.

4.2.9 Zinc (Zn)

Zinc		Isotopes				
Mass	1+	64	66	67	68	70
	2+	32	33	33,5	34	35
Abundance (%)		48,89	27,77	4,12	18,59	0,638
Fluorinated species	ZnF^+	83	85	86	87	89
	ZnF_2^+	102	104	105	106	108

The doubly charged state of Zn is used to confirm its presence in the sample. A line at mass 33,5 is due to the doubly charged species of ^{67}Zn. This line can, however, not be measured to quantify Zn as it is too light in intensity, because the abundance of ^{67}Zn is only 4,12%.

For Zn in the singly charged state, the line obtained for each of the isotopes appears as a doublet or a triplet which can be resolved. Most of the interferences at these masses are due to the fluorinated species of the other elements present in the sample.

The line at mass 64 is very dark in intensity and is due to the major isotope ^{64}Zn. The only possible interference is from $^{64}Ni^+$. Because this isotope of Ni has a low abundance (1,01%), it does not affect the measuring of the $^{64}Zn^+$ line.

At mass 66 a resolved triplet is obtained. The left-hand line is due to $^{66}Zn^+$ and the other two lines are due to $^{28}SiF_2{}^+$ and $^{47}TiF^+$ as interferences.

Similarly, for the line at mass 67, the left-hand line of the resolved triplet is due to $^{67}Zn^+$ and the other two lines are due to $^{29}SiF_2{}^+$, $^{48}TaF^+$ and $^{48}CaF^+$ as interferences.

The resolved triplet at mass 68 has one strong line and two weak lines. The left-hand line, which is the strong line, is due to $^{68}Zn^+$. The two weak lines are due to $^{30}SiF_2{}^+$ and $^{49}TiF^+$, where the abundance of ^{30}Si and ^{49}Ti is very small.

It is apparent from the above discussion that Zn can be measured at any of its isotopes up to mass 68, as long as the upper window is carefully chosen so as not to include the interfering adjacent lines.

The doublet at mass 70 is due to a number of species, apart from $^{70}Zn^+$. These possible interferences are $^{32}SF_2^+$, $^{51}VF^+$ and $^{13}CF_3^+$.

A weak line is obtained at mass 83, which is due to the fluorinated species of the main isotope of Zn, namely $^{64}ZnF^+$. No line is observed at mass 102 to confirm the presence of ZnF_2^+.

4.2.10 Yttrium (Y)

Yttrium		Isotopes
Mass	1+	89
	2+	44,5
Abundance (%)		100
Fluorinated species	YF^+	108
	YF_2^+	127
	YF_3^+	146

The single line at mass 44,5 is unique for the doubly charged ion of the mono-isotopic ^{89}Y. In the case of the singly charged ion, a doublet is obtained at mass 89, which can be resolved using mass-defect values. The strong left-hand line is due to $^{89}Y^+$ and the weak right-hand line is due to the fluorinated species of S, namely $^{32}SF_3^+$. The presence of this interference at mass 89 does not hinder the measuring of the Y line. Only the longest exposures are affected, which are in any case discarded as saturated points. The 50% transmission intercept obtained for the Y line is thus a true value for Y in the singly charged state.

In a UF_4/graphite matrix the internal standard, Y, also forms fluorinated species, i.e. YF^+. This is in contrast to the use of Y as an internal standard for a U_3O_8/graphite matrix. The difference obtained between the Y ratios, derived as the number of singly charged ions relative to the number of doubly charged ions, for the two types of matrices could be ascribed to the fact that Y also forms fluorinated species in a UF_4/graphite matrix.

The line obtained at mass 108 is due to $^{32}SF_4{}^+$ and $^{89}YF^+$. Similarly, the line at mass 127 is due to $^{32}SF_5{}^+$, $^{89}YF_2{}^+$ and $^{235}UF^{2+}$. No line is obtained at mass 146 to confirm the presence of $YF_3{}^+$.

4.2.11 Uranium (U)

Apart from the normal fingerprint spectrum of uranium up to charge state 5, a number of other lines are also observed. The fingerprint spectrum of U is given in Table 4.1. on page 38. A strong line at mass 128,5 is due to the doubly charged ion of the fluorinated species of the major isotope of uranium, namely $^{238}UF^{2+}$. The line at mass 127 could be as a result of the combination of $^{235}UF^{2+}$ with $^{32}SF_5{}^+$ and $^{89}YF_2{}^+$. A weak line at mass 85,67 is due to the triply charged ion of fluorinated ^{238}U, namely $^{238}UF^{3+}$.

The line observed at mass 125 is of interest as it can be related to the formation of a UC^+ species. It would appear that the UF_4 molecule is in this case totally stripped of its fluoride ions within the plasma, leaving the U^+ ion which recombines with a C^+ ion, forming a UC^+ species. At mass 125 the doubly charged species $^{238}UC^{2+}$ is observed.

4.2.12 Selection of isotopes and charge states

A summary of the isotopes and charge states used to quantify each of the seven impurity elements in the UF_4/graphite matrix is given in Table 4.3.

Table 4.3: Isotopes and charge states used to quantify impurity elements in a UF_4/graphite matrix

Element	Charge state	m/e	Isotope	Abundance (%)
Al	2+	13,5	27	100
P	2+	15,5	31	100
Ca	2+ 2+	20 21	40 42	96,94 0,65
Si	1+	30	30	3,09
S	1+	32	32	95,0
Cl	1+ 1+	35 37	35 37	75,72 24,28
Zn	1+ 1+	64 67	64 67	48,89 27,77
Y	1+ 2+	89 44,5	89 89	100 100