ceramics

MDPI

Supplementary

Table A. Standardless SEM analysis of microprobe standards.

Fe_2O_3								**Rutile**							
Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff	Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff
O	0.11279	29.24	0.46	59.05	30.06	−0.82	−3	O	0.0396	40.97	0.8	67.51	40.05	0.92	2
Fe	0.36553	70.76	0.46	40.95	69.94	0.82	1	Ti	0.3514	59.03	0.8	32.49	59.95	−0.92	−2
Total:		100		100				Total:		100		100			
Cr_2O_3								**MgO**							
Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff	Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff
O	0.14046	32.66	0.41	61.19	31.58	1.08	3	O	0.09198	38.02	0.37	48.24	39.7	−1.68	−4
Cr	0.33735	67.34	0.41	38.81	68.42	-1.08	−2	Mg	0.20483	61.98	0.37	51.76	60.3	1.68	3
Total:		100		100				Total:				100			
Rhodonite								**Orthoclase**							
Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff	Element	k Ratio	Mass %	St dev	Atom %	Std Mass %	Difference	% Diff
O	0.09954	38.63	0.49	60.51	37.77	0.86	2	O	0.0815	46.27	0.46	61.43	46.47	−0.2	0
Mg	0.00403	1.33	0.13	1.37	1.12	0.21	19	Na	0.00278	1.02	0.12	0.95	1.01	0.01	1
Si	0.09762	22.62	0.33	20.18	22.11	0.51	2	Al	0.04005	9.99	0.21	7.86	9.81	0.18	2
Ca	0.02689	5.09	0.2	3.19	5.1	−0.01	0	Si	0.12658	30.8	0.35	23.29	30.4	0.4	1
Mn	0.15333	32.33	0.55	14.75	32.85	−0.52	−2	K	0.05287	11.92	0.27	6.47	12.18	−0.26	−2
Total:		100		100				Total:				100		100	

Table B. Formula calculation of Spinel A in sample CMD0.

				Cr-spinel Formula Calculation					
Oxide	**Percent**	**Mol Mass**	Mole Prop	No Cations	Cations to 3	Oxygens to 4	Cations recalc	Oxides Recalc	Recalc %
TiO_2	0.12625	79.88	0.0016	0.0016	0.0028	0.0056	0.0028	0.0015805	0.13
Al_2O_3	9.26375	101.96	0.0909	0.1817	0.3245	0.4867	0.3245	0.09085671	9.26
Cr_2O_3	26.76375	151.99	0.1761	0.3522	0.6289	0.9433	0.6289	0.17608889	26.76
Fe_2O_3	35.77688	159.69	0.2240	0.4481	0.8001		1.0410	0.29149952	46.55
FeO		71.85			0.0000	1.3206	−0.2409	−0.13491995	−9.69
MgO	28.07	40.3	0.6965	0.6965	1.2437	1.2437	1.2437	0.69652605	28.07
Total	100.00			1.6801	3.0000	4.0000	3.0000		101.08
					xFe2+ + yFe3+ =	0.8001			
					xFe2+ + 1.5yFe3+ =	1.3206	Determined by difference		
					0.5yFe3+ =	0.5205			
					Fe3+ =	1.0410			

Table C. Comparison between bulk compositions calculated from XRD and EDS analysis and ICP analysis.

	SiO2	**CaO**	**TiO2**	**Al2O3**	**Cr2O3**	**Fe2O3**	**MgO**
			CMD0				
Calc Analysis	3.84	1.42	0.28	11.58	26.93	13.18	42.91
ICP Analysis	2.34	0.77	0.28	9.65	26.40	12.60	44.65
			CMD1				
Calc Analysis	3.11	1.34	2.61	8.34	23.31	15.80	45.50
ICP Analysis	2.31	0.89	1.21	8.72	25.79	12.11	45.55
			CMD3				
Calc Analysis	2.10	0.77	5.24	8.01	22.97	16.63	44.30
ICP Analysis	1.81	0.65	3.88	8.03	23.45	12.35	45.35
			CMD5				
Calc Analysis	2.44	0.92	8.56	9.22	23.22	12.18	43.49
ICP Analysis	2.05	0.79	4.88	8.40	23.89	11.67	45.25
			CMD7				
Calc Analysis	3.86	1.09	4.70	7.98	23.69	15.72	42.99
ICPAnalysis	2.93	0.99	6.87	8.48	22.33	12.03	44.00

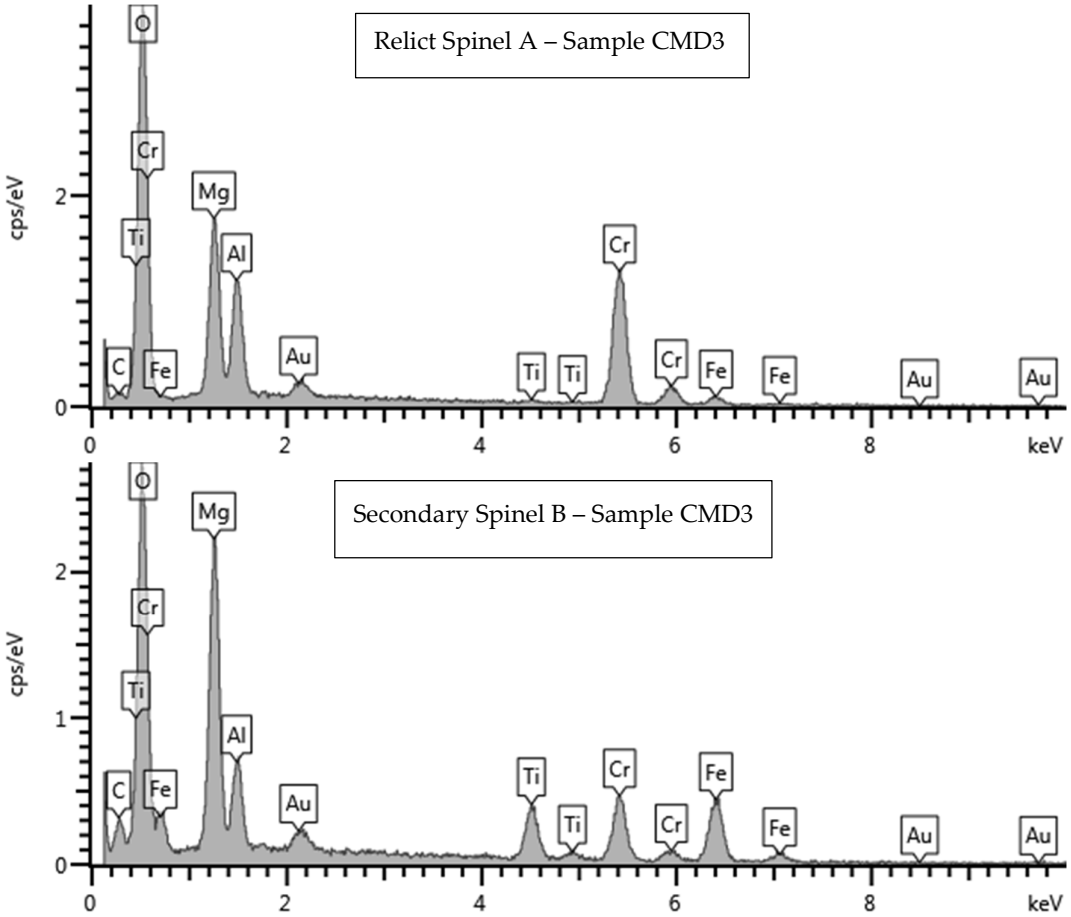
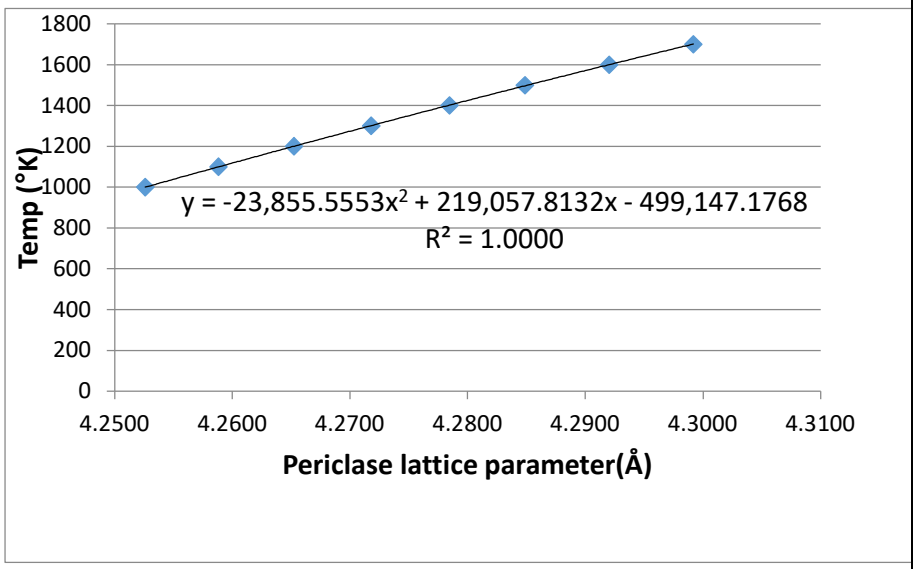
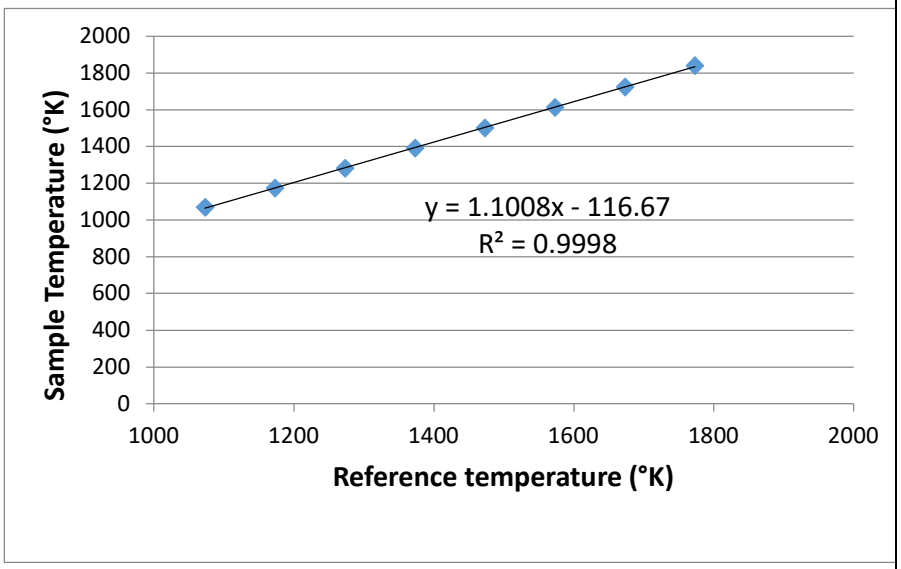


Figure A. EDS spectra of Spinel A (**top**) and spinel B (**bottom**) from sample CMD3.

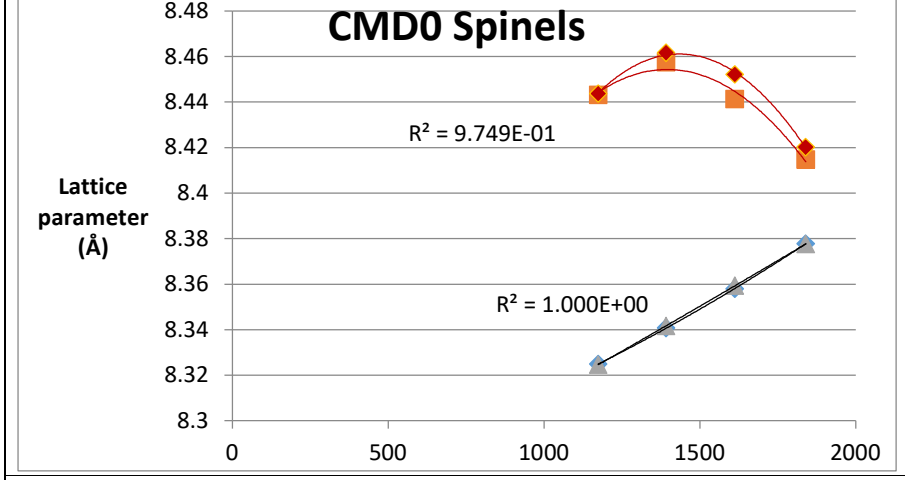


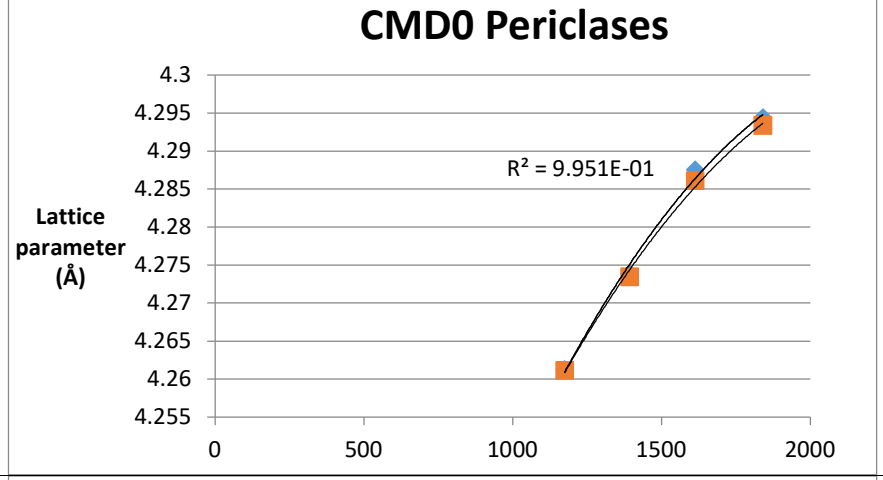
(a)

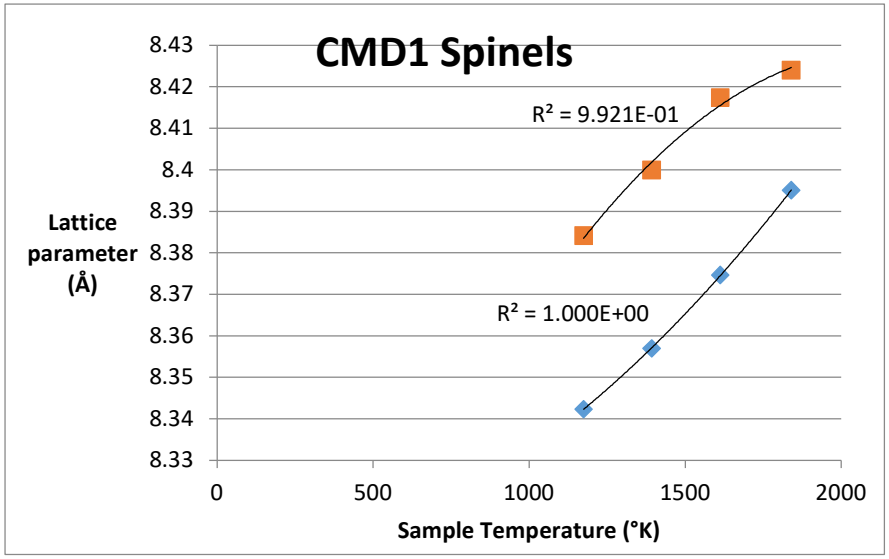


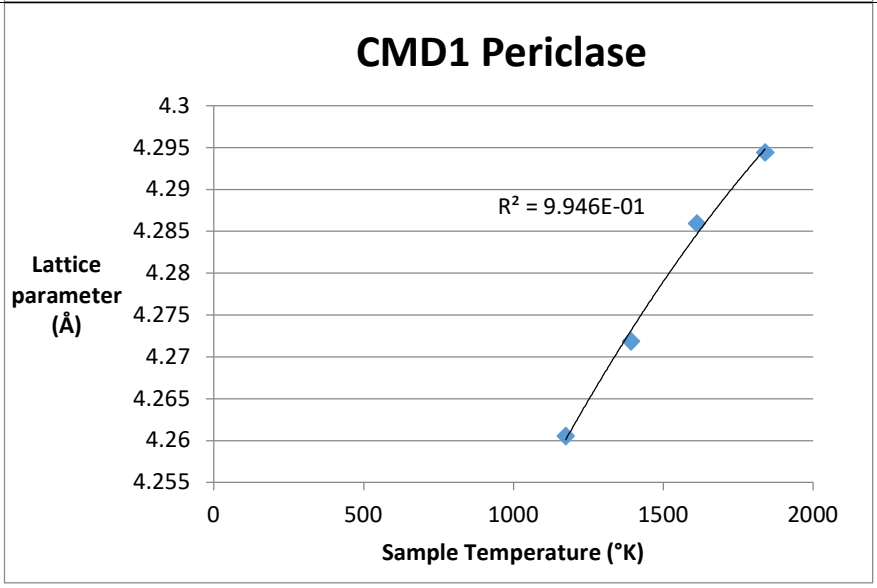
(b)

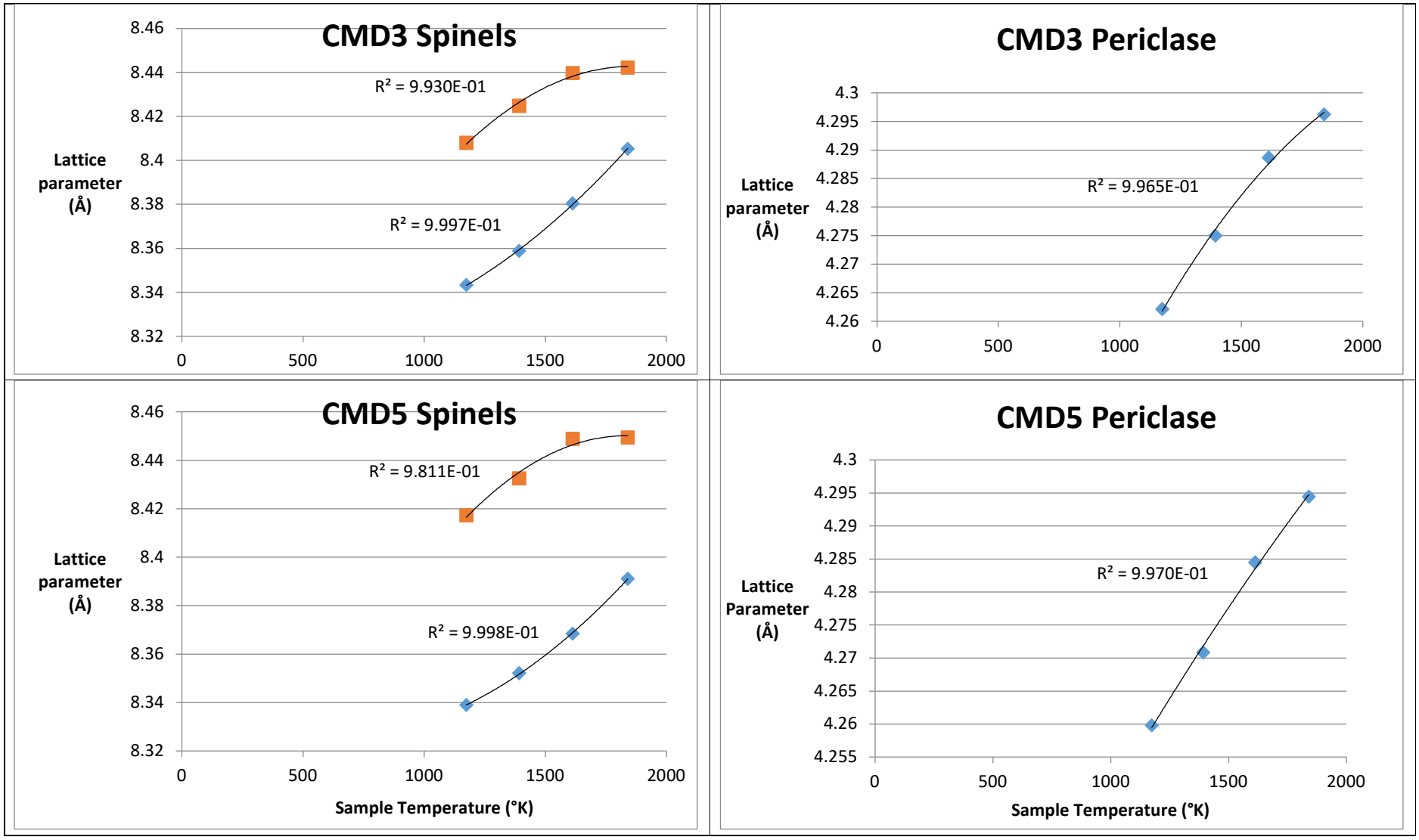
Figure B. (**a**) Variation of the periclase lattice parameter with temperature from the data of Toloukian et al [21] and (**b**) the corrected sample temperature as calibrated from high temperature XRD data of MgO.


CMD0 Spinels
Lattice parameter (Å)
R² = 9.749E-01
R² = 1.000E+00
8.48
8.46
8.44
8.42
8.4
8.38
8.36
8.34
8.32
8.3
0
500
1000
1500
2000


CMD0 Periclases
Lattice parameter (Å)
R² = 9.951E-01
4.3
4.295
4.29
4.285
4.28
4.275
4.27
4.265
4.26
4.255
0
500
1000
1500
2000


CMD1 Spinels
Lattice parameter (Å)
R² = 9.921E-01
R² = 1.000E+00
8.43
8.42
8.41
8.4
8.39
8.38
8.37
8.36
8.35
8.34
8.33
0
500
1000
1500
2000
Sample Temperature (°K)


CMD1 Periclase
Lattice parameter (Å)
R² = 9.946E-01
4.3
4.295
4.29
4.285
4.28
4.275
4.27
4.265
4.26
4.255
0
500
1000
1500
2000
Sample Temperature (°K)


CMD3 Spinels
R² = 9.930E-01
R² = 9.997E-01
Lattice parameter (Å)
8.46
8.44
8.42
8.4
8.38
8.36
8.34
8.32
0
500
1000
1500
2000
CMD3 Periclase
R² = 9.965E-01
Lattice parameter (Å)
4.3
4.295
4.29
4.285
4.28
4.275
4.27
4.265
4.26
CMD5 Spinels
R² = 9.811E-01
R² = 9.998E-01
Lattice parameter (Å)
Sample Temperature (°K)
CMD5 Periclase
R² = 9.970E-01
Lattice Parameter (Å)
4.255
Sample Temperature (°K)

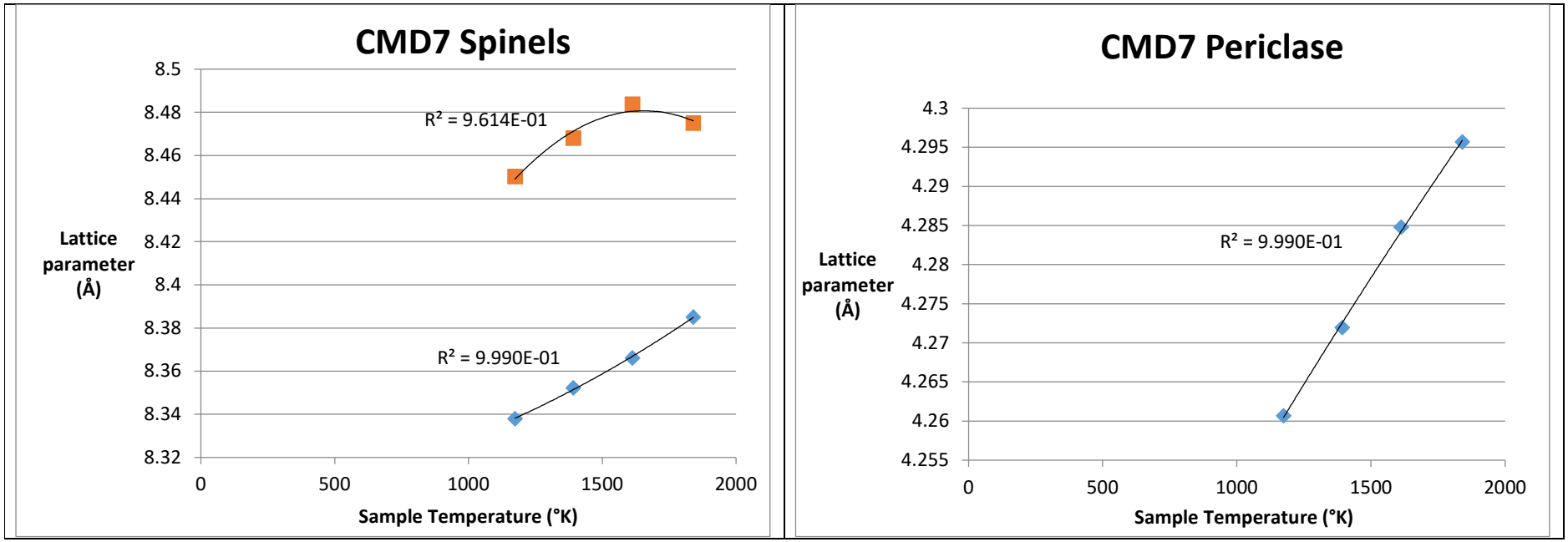


Figure C. Thermal expansion data for CMD samples. All diagrams show lattice constant as a function of temperature in degrees Kelvin.