Electrochemistry of a series of symmetric and asymmetric CpNiBr(NHC) complexes: Probing the electrochemical environment due to push-pull effects

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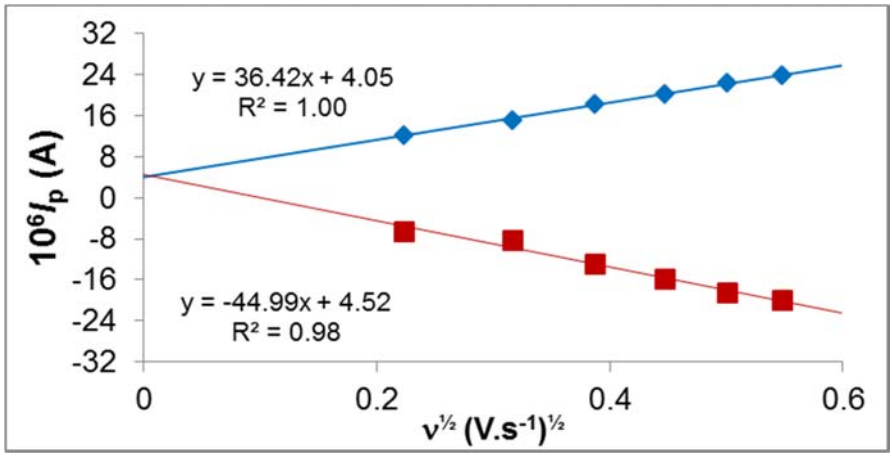
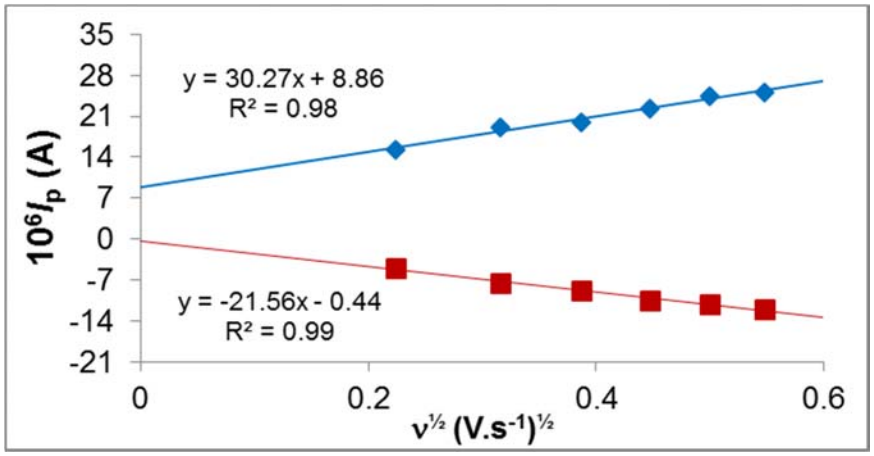
Supplementary Information

1 Graphs of 1-9 (region II): $v^{½}$ vs. I_{pa} (NiII/NiIII oxidation blue) and I_{pc} (NiIII/NiII reduction red)

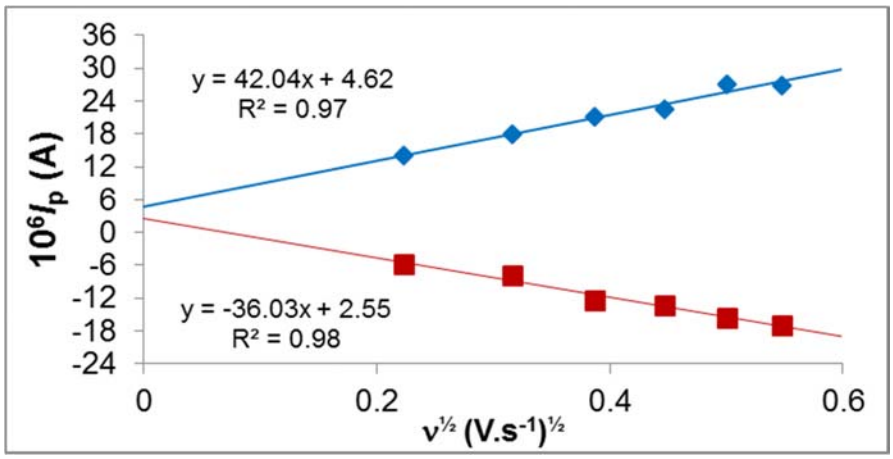
Complex **1**



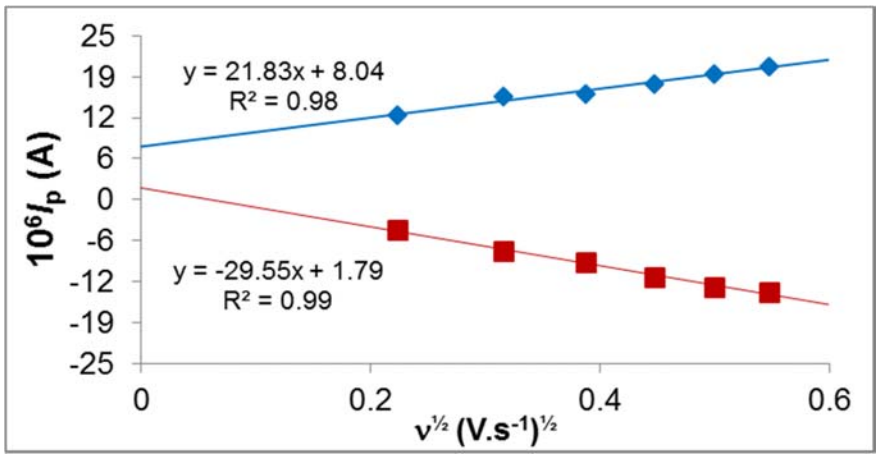
Complex **2**



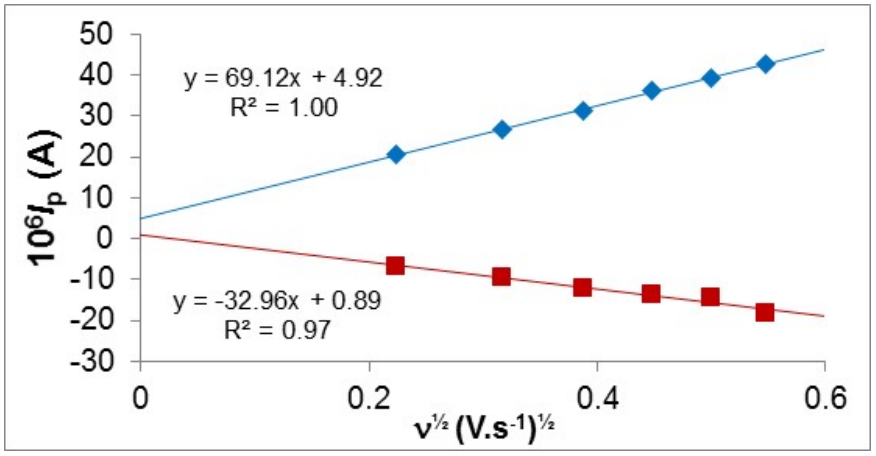
Complex **3**



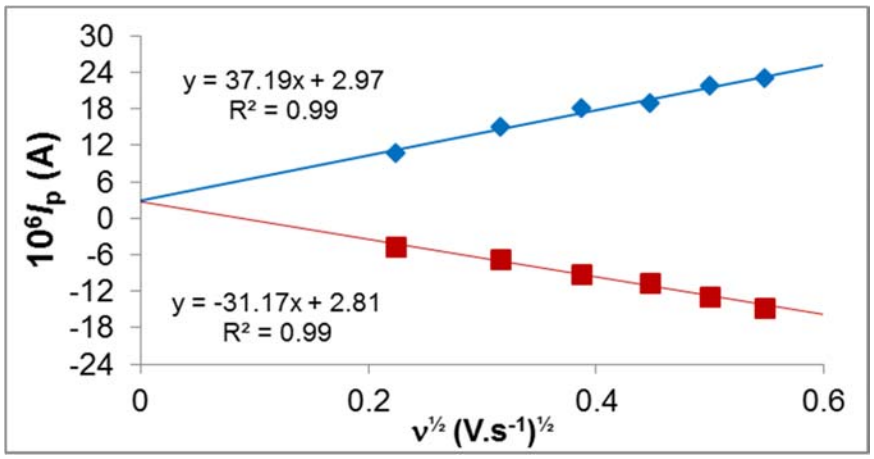
Complex 4



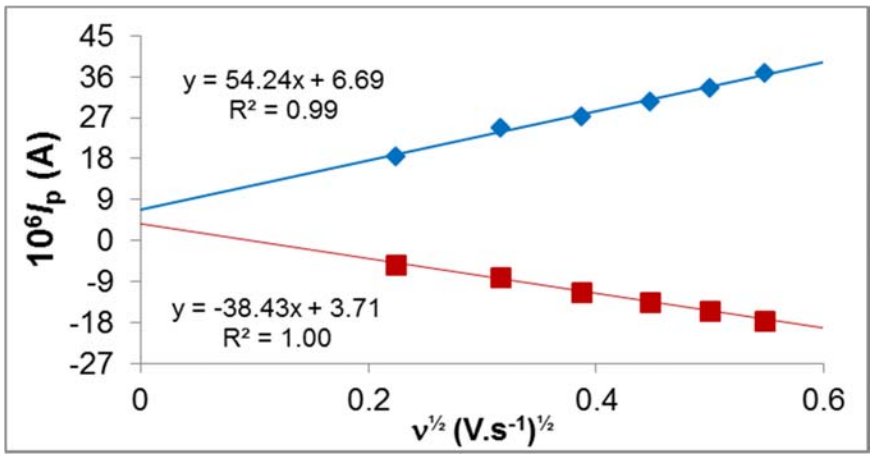
Complex 5



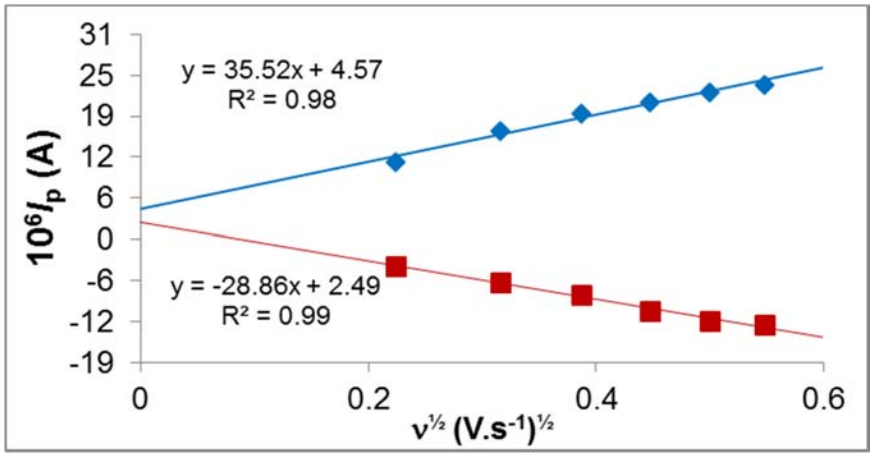
Complex **6**



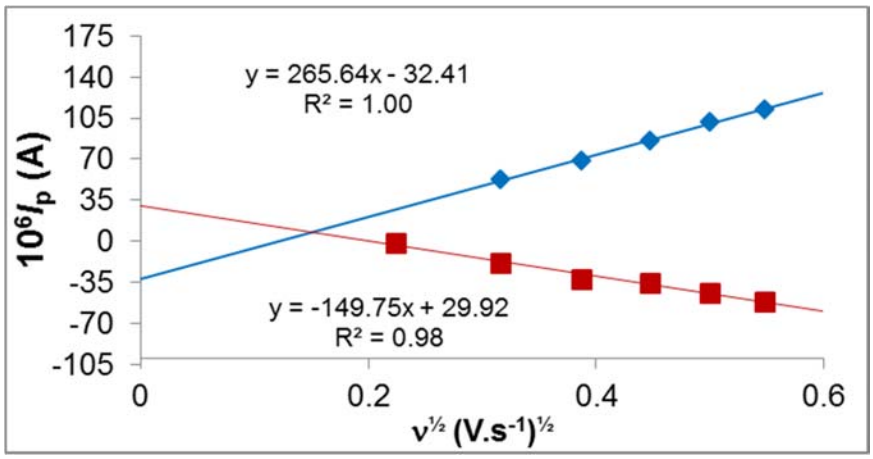
Complex **7**



Complex **8**



Complex **9**


y = 265.64x - 32.41
R² = 1.00
y = -149.75x + 29.92
R² = 0.98
10⁶Ip (A)
ν½ (V.s-1)½
175
140
105
70
35
0
-35
-70
-105
0
0.2
0.4
0.6

2 Tables of 1-9 (region II) with electrochemical data

Complex **1**: (old 2)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.229E-05	6.473E-06	0.53	0.0125	0.0995	0.087	0.056
0.10	1.520E-05	8.235E-06	0.54	0.0135	0.0995	0.086	0.057
0.15	1.842E-05	1.289E-05	0.70	0.0115	0.1005	0.089	0.056
0.20	2.039E-05	1.579E-05	0.77	0.0105	0.1015	0.091	0.056
0.25	2.237E-05	1.847E-05	0.83	0.0095	0.1025	0.093	0.056
0.30	2.383E-05	2.000E-05	0.84	0.0085	0.1035	0.095	0.056
0.50	2.857E-05	2.667E-05	0.93	0.0045	0.1035	0.099	0.054
1.00	3.667E-05	3.424E-05	0.93	0.0015	0.1035	0.102	0.053
5.00	7.118E-05	6.353E-05	0.89	-0.0065	0.1065	0.113	0.050

Complex **5**: (old 1)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	2.050E-05	1.294E-06	0.33	0.0145	0.1265	0.112	0.071
0.10	2.662E-05	2.977E-06	0.35	0.0205	0.1315	0.111	0.076
0.15	3.145E-05	4.412E-06	0.39	0.0195	0.1365	0.117	0.078
0.20	3.628E-05	5.471E-06	0.38	0.0175	0.1385	0.121	0.078
0.25	3.930E-05	5.941E-06	0.37	0.0165	0.1425	0.126	0.080
0.30	4.279E-05	6.933E-06	0.40	0.0145	0.1445	0.130	0.080
0.50	5.118E-05	7.583E-06	0.46	0.0085	0.1495	0.141	0.079
1.00	6.400E-05	1.145E-06	0.46	0.0025	0.1545	0.152	0.079
5.00	8.968E-05	1.093E-06	0.65	0.0055	0.1375	0.132	0.072

Complex **3**: (old 3 – reg)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.398E-05	5.763E-06	0.41	0.0265	0.1095	0.083	0.068
0.10	1.795E-05	7.841E-06	0.44	0.0255	0.1105	0.085	0.068
0.15	2.103E-05	1.235E-05	0.59	0.0305	0.1135	0.083	0.072
0.20	2.257E-05	1.343E-06	0.59	0.0285	0.1155	0.087	0.072
0.25	2.710E-05	1.565E-06	0.58	0.0265	0.1155	0.089	0.071
0.30	2.692E-05	1.692E-05	0.63	0.0265	0.1165	0.090	0.072
0.50	3.316E-05	2.605E-05	0.79	0.0255	0.1195	0.094	0.073
1.00	4.290E-05	3.355E-05	0.78	0.0175	0.1205	0.103	0.069
5.00	7.419E-05	6.323E-05	0.85	0.0065	0.1265	0.120	0.067

Complex **6**: (old 4)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.085E-05	4.545E-06	0.42	0.0425	0.1305	0.088	0.087
0.10	1.500E-05	6.800E-06	0.45	0.0445	0.1315	0.087	0.088
0.15	1.814E-05	9.186E-06	0.51	0.0405	0.1325	0.092	0.087
0.20	1.908E-05	1.053E-05	0.55	0.0395	0.1355	0.096	0.088
0.25	2.182E-05	1.288E-05	0.59	0.0385	0.1365	0.098	0.088
0.30	2.303E-05	1.470E-05	0.64	0.0375	0.1375	0.100	0.088
0.50	2.780E-05	1.900E-05	0.68	0.0305	0.1385	0.108	0.085
1.00	3.474E-05	2.842E-05	0.82	0.0285	0.1365	0.108	0.083
5.00	5.842E-05	4.000E-05	0.68	0.0085	0.1465	0.138	0.078

Complex **2**: (old 5)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.533E-05	4.917E-06	0.32	0.0125	0.1165	0.104	0.065
0.10	1.919E-05	7.568E-06	0.39	0.0125	0.1235	0.111	0.068
0.15	2.000E-05	8.837E-06	0.44	0.0125	0.1305	0.118	0.072
0.20	2.227E-05	1.045E-05	0.47	0.0115	0.1335	0.122	0.073
0.25	2.450E-05	1.117E-05	0.46	0.0085	0.1345	0.126	0.072
0.30	2.516E-05	1.194E-05	0.47	0.0075	0.1365	0.129	0.072
0.50	4.088E-05	1.618E-05	0.40	-0.0005	0.1425	0.143	0.071
1.00	4.667E-05	2.067E-05	0.44	-0.0055	0.1365	0.142	0.066
5.00	8.061E-05	2.727E-05	0.34	-0.0255	0.1435	0.169	0.059

Complex **7**: (old 6)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.850E-05	5.200E-06	0.28	0.0455	0.1315	0.086	0.089
0.10	2.485E-05	8.030E-06	0.32	0.0515	0.1335	0.082	0.093
0.15	2.727E-05	1.121E-05	0.41	0.0525	0.1375	0.085	0.095
0.20	3.054E-05	1.339E-05	0.44	0.0515	0.1405	0.089	0.096
0.25	3.349E-05	1.535E-05	0.46	0.0505	0.1445	0.094	0.098
0.30	3.690E-05	1.762E-05	0.48	0.0495	0.1455	0.096	0.098
0.50	4.333E-05	2.182E-05	0.50	0.0455	0.1515	0.106	0.099
1.00	5.680E-05	3.400E-05	0.60	0.0405	0.1525	0.112	0.097
5.00	9.754E-05	5.328E-05	0.55	0.0235	0.1595	0.136	0.092

Complex **4**: (old 7)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.279E-05	4.643E-06	0.36	0.0295	0.1205	0.091	0.075
0.10	1.558E-05	7.791E-06	0.50	0.0305	0.1215	0.091	0.076
0.15	1.600E-05	9.400E-06	0.59	0.0295	0.1285	0.099	0.079
0.20	1.750E-05	1.171E-05	0.67	0.0275	0.1285	0.101	0.078
0.25	1.908E-05	1.329E-05	0.70	0.0265	0.1305	0.104	0.079
0.30	2.017E-05	1.400E-05	0.69	0.0245	0.1315	0.107	0.078
0.50	2.380E-05	1.860E-05	0.78	0.0195	0.1295	0.110	0.075
1.00	2.897E-05	2.538E-05	0.88	0.0175	0.1175	0.100	0.068
5.00	5.070E-05	3.256E-05	0.64	0.0055	0.1165	0.111	0.061

Complex **8**:(old 8)

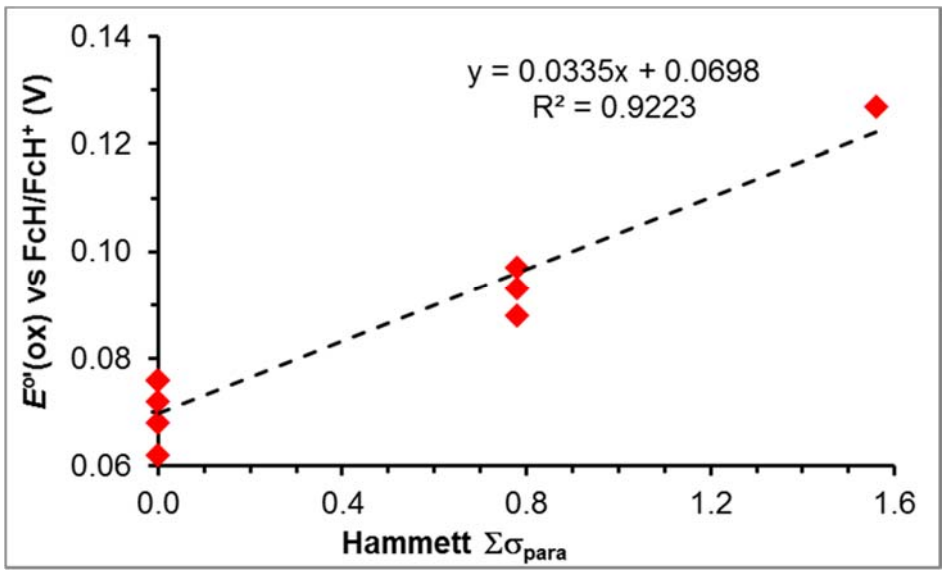
Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	1.165E-05	4.000E-06	0.34	0.0535	0.1405	0.087	0.097
0.10	1.640E-05	6.512E-06	0.40	0.0535	0.1395	0.086	0.097
0.15	1.907E-05	8.372E-06	0.44	0.0535	0.1435	0.090	0.099
0.20	2.076E-05	1.091E-05	0.53	0.0525	0.1475	0.095	0.100
0.25	2.227E-05	1.227E-05	0.55	0.0525	0.1495	0.097	0.101
0.30	2.333E-05	1.288E-05	0.55	0.0495	0.1505	0.101	0.100
0.50	2.640E-05	1.720E-05	0.65	0.0455	0.1535	0.108	0.100
1.00	3.316E-05	2.368E-05	0.71	0.0425	0.1485	0.106	0.100
5.00	6.158E-05	3.895E-05	0.63	0.0315	0.1505	0.119	0.091

Complex **9**: (old 9)

Scan rate; υ ($V.s^{-1}$)	I_{pa} (A)	I_{pc} (A)	I_{pc}/I_{pa}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	E°' (V)
0.05	6.200E-06	1.267E-06	0.20	0.0615	0.1665	0.105	0.114
0.10	5.267E-05	1.867E-05	0.35	0.0655	0.1735	0.108	0.120
0.15	6.867E-05	3.200E-05	0.47	0.0735	0.1695	0.096	0.122
0.20	8.600E-05	3.600E-05	0.42	0.0755	0.1715	0.096	0.124
0.25	1.021E-05	4.357E-05	0.43	0.0725	0.1715	0.099	0.122
0.30	1.125E-05	5.167E-05	0.46	0.0735	0.1715	0.098	0.123
0.50	1.221E-05	6.047E-06	0.50	0.0735	0.1745	0.101	0.124
1.00	1.697E-05	1.197E-05	0.71	0.0695	0.1815	0.112	0.126
5.00	2.618E-05	1.618E-05	0.62	0.0655	0.1875	0.122	0.127

3 Figure S1: $E^{\circ\prime}$ versus $\Sigma\sigma_{para}$

Relationship between the formal reduction potential, $E^{\circ\prime}$, of the Ni^{II}/Ni^{III} redox couple and the sum of the Hammett constants of the *para*-substituents on the phenyl ring of the *N*-substituents (benzyl, phenethyl, 4-NO_2-benzyl).



4 Optimized coordinates (DFT calculations) of 1-9

All of the following optimized coordinates are based on calculations of nickel in the singlet multiplicity (lowest energy) and lowest energy conformers (see manuscript for details).

Complex 1 (neutral):

Br	0.96148000	-1.17166200	-1.79984400
N	-0.87983800	1.37812100	0.52134200
C	-2.84902600	-0.12294600	0.78051000
C	-2.82041400	-0.83538700	-0.42444800
C	-1.56689400	0.40837800	1.38477300
C	-3.99952700	-1.33890600	-0.96413700
C	-4.06933900	0.07171300	1.43020600
C	-5.21618500	-1.14195000	-0.30985100
C	-5.25006000	-0.43690800	0.88950400
C	0.38280400	1.22327300	0.04959600
C	-1.44540200	2.55418000	0.04880400
C	2.23416300	0.02557800	2.28813900
C	1.98977300	-1.36543400	2.15927900
C	2.83931000	-1.82957700	1.13425500
H	1.74378300	0.69639300	2.97927800
H	-0.84784200	-0.39539800	1.54876000
H	-4.09895900	0.61830400	2.36801800
H	-1.77211800	0.88166200	2.34902700
H	-6.19126100	-0.28129800	1.40481900

H	-3.96700600	-1.89219100	-1.89591500
H	1.23534000	-1.93809400	2.67666300
H	-2.44975200	2.85056300	0.29575100
H	-1.87513200	-0.99568800	-0.93472400
H	2.85609700	-2.83050400	0.72958100
H	-6.13206100	-1.53873600	-0.73338000
N	0.60698900	2.32355700	-0.70911900
C	-0.50945800	3.14702500	-0.72833100
H	-0.53785800	4.06749400	-1.28554300
C	3.37798600	0.37042200	1.46445600
C	3.74229800	-0.76860000	0.75744800
H	3.83514500	1.34716100	1.40554800
H	4.51903100	-0.84649300	0.01165400
C	1.80052900	2.52071000	-1.52476600
H	2.00628500	3.58799400	-1.61430400
H	2.63711200	2.02243800	-1.04027500
Ni	1.56418400	-0.25802300	0.28367800
H	1.65681600	2.07803900	-2.51161100

Complex 1 (cation, oxidized):

Br	1.13351200	-1.41543900	-1.61121300
N	-0.91487700	1.17845100	0.30997800
C	-2.94972700	-0.20839300	0.70538500
C	-3.13099100	-0.93069300	-0.47981100
C	-1.56157900	0.15888000	1.17124600

C	-4.41170700	-1.27130100	-0.90109100
C	-4.06423500	0.16132500	1.46165100
C	-5.52141500	-0.89753300	-0.14221500
C	-5.34750800	-0.18308300	1.03951000
C	0.36380600	1.14501300	-0.11456300
C	-1.54986000	2.30745200	-0.18499800
C	2.02682000	-0.03327700	2.36729400
C	2.29689900	-1.37309500	2.03297900
C	3.34589900	-1.37652900	1.06403500
H	1.28049000	0.31835100	3.06340200
H	-0.90122900	-0.70894800	1.15751300
H	-3.93247100	0.71149000	2.38807600
H	-1.59391400	0.54875000	2.19138200
H	-6.20638800	0.10342000	1.63462100
H	-4.54584900	-1.83397500	-1.81733700
H	1.76280000	-2.24238600	2.38669800
H	-2.58585100	2.51479300	0.01751200
H	-2.27016700	-1.22798700	-1.07003100
H	3.74792600	-2.25104200	0.57489700
H	-6.51795500	-1.16785500	-0.47073300
N	0.53863700	2.24060700	-0.88252400
C	-0.63779900	2.97430600	-0.93137600
H	-0.72114500	3.88726700	-1.49536700
C	2.95663000	0.80329200	1.63921700
C	3.79135300	-0.03657900	0.87354900

H	3.01657600	1.87887200	1.70955900
H	4.57915300	0.27894100	0.20607400
C	1.77238600	2.59839700	-1.58427900
H	1.52081200	3.20875800	-2.44982200
H	2.43876600	3.16282700	-0.92977500
Ni	1.69110500	-0.22479800	0.25479000
H	2.26442300	1.69093000	-1.92973500

Complex 1 (anion, reduced):

Br	-1.41813500	0.80423400	2.22391900
N	0.91229000	0.89092300	-1.57627700
C	2.63964900	-0.48945800	-0.44248000
C	2.22410000	-0.38586100	0.89149500
C	1.62232300	-0.38789600	-1.56277400
C	3.15446300	-0.49336100	1.92026800
C	3.99093300	-0.70663500	-0.71908100
C	4.50384900	-0.71108800	1.63740000
C	4.92214500	-0.81955600	0.31394800
C	-0.33588100	1.05613000	-1.04031100
C	1.45761400	2.09473100	-2.00051900
C	-1.36172800	-2.70386200	-1.83442800
C	-1.00043700	-3.06308800	-0.51783200
C	-1.97927300	-2.54414500	0.36541100
H	-0.80291800	-2.93695700	-2.73430400
H	0.85479800	-1.15952900	-1.45547900

H	4.31855800	-0.79287200	-1.75159500
H	2.11198000	-0.52486400	-2.53173300
H	5.96911800	-0.98942700	0.08323400
H	2.81531100	-0.40853700	2.94684500
H	-0.11895500	-3.62143200	-0.22614800
H	2.44583500	2.17099700	-2.42125700
H	1.17571100	-0.21836300	1.12535600
H	-2.00813100	-2.67472200	1.43816100
H	5.22391300	-0.79639900	2.44503700
N	-0.55285000	2.39737000	-1.16366700
C	0.52618800	3.04481100	-1.74607200
H	0.53937000	4.10713700	-1.92388600
C	-2.56494900	-1.96199100	-1.77983100
C	-2.96592900	-1.87501800	-0.41673000
H	-3.11010300	-1.56440300	-2.62697800
H	-3.89721100	-1.46459400	-0.04838500
C	-1.77434400	3.04522100	-0.70211000
H	-1.57235000	4.10461300	-0.53050800
H	-2.57047800	2.94154600	-1.44451100
Ni	-1.44765900	-0.30373600	-0.12269600
H	-2.07369200	2.57254900	0.23597400

Complex 2 (neutral):

Ni	0.04435400	1.07738900	0.60798000
Br	-0.15176000	0.73800400	-1.71691800

C	0.03181400	-0.79230300	1.00763500
C	0.69320400	-2.91506200	1.41050100
C	-0.66068500	-2.90377600	1.41505800
H	1.39070100	-3.71930200	1.56944200
H	-1.36929600	-3.69688200	1.58005900
C	0.31594900	3.25218100	0.70510600
C	-1.00634000	3.01746100	1.23187300
C	1.26618800	2.66229300	1.56666800
H	0.53700000	3.83755700	-0.17496100
C	-0.87826500	2.18718900	2.33774700
H	-1.92642800	3.37626300	0.79589000
C	0.53586200	1.90399100	2.51357400
H	2.33963000	2.70233700	1.46250800
H	-1.67562500	1.79673500	2.95283500
H	0.95393700	1.31224800	3.31546100
N	-1.04988800	-1.59437000	1.17011900
N	1.10147700	-1.61155800	1.16482100
C	-2.43434300	-1.15026900	0.98638100
H	-3.03222100	-1.50676500	1.82971000
H	-2.41285000	-0.06189600	1.01929900
C	-3.02845500	-1.62695400	-0.35158000
H	-2.34015500	-1.32919900	-1.14586700
H	-3.09241300	-2.71983300	-0.35633500
C	-4.39438600	-1.02460500	-0.59280500
C	-5.55906900	-1.67124700	-0.16778200

C	-4.50977100	0.21864300	-1.22605600
C	-6.81079600	-1.09211900	-0.36720200
H	-5.48736100	-2.64176500	0.31449400
C	-5.75973700	0.79892600	-1.42669700
H	-3.61206000	0.72324200	-1.56941400
C	-6.91387400	0.14613800	-0.99686500
H	-7.70439000	-1.61016300	-0.03662700
H	-5.83262200	1.75900600	-1.92560000
H	-7.88706500	0.59661000	-1.15686500
C	2.49007800	-1.18922300	0.96899800
H	2.51255400	-0.11202200	1.12979400
H	3.10832900	-1.66224200	1.73636600
C	3.01002700	-1.52264000	-0.44178900
H	3.00867700	-2.60830700	-0.58216300
H	2.31292400	-1.09533400	-1.16694100
C	4.40031200	-0.96920400	-0.65802900
C	5.53653700	-1.71692900	-0.33257500
C	4.57244200	0.32619800	-1.15948500
C	6.81364500	-1.18540600	-0.49874800
H	5.42162100	-2.72862500	0.04529600
C	5.84794200	0.86017200	-1.32644400
H	3.69875100	0.91053000	-1.43006300
C	6.97243500	0.10659500	-0.99493700
H	7.68365100	-1.78173900	-0.24653000
H	5.96351200	1.86295900	-1.72258900

H	7.96547800	0.52076900	-1.12839500

Complex 2 (cation, oxidized):

Ni	0.00002100	1.15972600	0.53976700
Br	0.00002100	0.89533100	-1.73062600
C	-0.00000500	-0.75634500	0.87130900
C	0.67717900	-2.86336300	1.20604100
C	-0.67724200	-2.86334000	1.20607900
H	1.37965000	-3.66700700	1.34410700
H	-1.37973300	-3.66696100	1.34417600
C	0.00008800	3.32269900	0.74435800
C	-1.15824400	2.81753400	1.40636600
C	1.15836500	2.81745700	1.40640000
H	0.00012100	3.99188900	-0.10285400
C	-0.72380500	1.92511700	2.40578600
H	-2.18260100	3.02721200	1.13653500
C	0.72383600	1.92506800	2.40580700
H	2.18274400	3.02706700	1.13659900
H	-1.34961600	1.35989000	3.07992500
H	1.34959000	1.35979700	3.07996200
N	-1.08128500	-1.55281000	0.99765000
N	1.08125500	-1.55283500	0.99767100
C	-2.48397900	-1.12512700	0.85734900
H	-3.04041900	-1.49863300	1.71967600
H	-2.49030700	-0.03670800	0.90459400

C	-3.12976800	-1.59799700	-0.45642700
H	-2.51371700	-1.25732100	-1.29212600
H	-3.14062200	-2.69153200	-0.48458700
C	-4.53750300	-1.05639600	-0.58386600
C	-5.61907800	-1.72757000	-0.00453600
C	-4.77446300	0.14539300	-1.25936400
C	-6.90817700	-1.20804900	-0.09431300
H	-5.45779700	-2.67176000	0.50699800
C	-6.06322900	0.66615400	-1.35168300
H	-3.94820700	0.66598800	-1.73409100
C	-7.13258000	-0.00859100	-0.76679000
H	-7.73785500	-1.74430700	0.35144000
H	-6.23415400	1.59109800	-1.89041800
H	-8.13649800	0.39192900	-0.84375700
C	2.48396000	-1.12518500	0.85738100
H	2.49031900	-0.03676900	0.90468000
H	3.04040000	-1.49875000	1.71968200
C	3.12971800	-1.59800500	-0.45642800
H	3.14055900	-2.69153800	-0.48463600
H	2.51365500	-1.25728400	-1.29210000
C	4.53745600	-1.05641200	-0.58387100
C	5.61903600	-1.72762400	-0.00459500
C	4.77441500	0.14540600	-1.25931700
C	6.90813900	-1.20811200	-0.09437400
H	5.45775600	-2.67183700	0.50689800

C	6.06318300	0.66615900	-1.35163800
H	3.94815400	0.66603200	-1.73400200
C	7.13254000	-0.00862400	-0.76679900
H	7.73782100	-1.74440000	0.35133600
H	6.23410700	1.59112700	-1.89033200
H	8.13646100	0.39188900	-0.84376700

Complex 2 (anion, reduced):

Ni	0.06804500	1.03414200	0.57615600
Br	-0.50109000	0.62408700	-1.91765700
C	-0.05587200	-0.85504900	1.16655400
C	0.50283000	-3.00912700	1.67031600
C	-0.84996500	-2.92982700	1.68713500
H	1.16089600	-3.84000800	1.86307600
H	-1.59421100	-3.67879900	1.90013800
C	1.83771500	3.00772400	0.78976300
C	0.45261300	3.28999900	0.66325500
C	2.05778900	2.42738300	2.05770900
H	2.59157600	3.21385700	0.04018600
C	-0.18695900	2.87952200	1.86973000
H	-0.02340500	3.78003300	-0.17428100
C	0.81118800	2.33312500	2.72006300
H	3.01186300	2.09231500	2.44773000
H	-1.22593700	3.04127900	2.12655800
H	0.64414800	1.92601400	3.70981900

N	-1.17100500	-1.61260600	1.38544500
N	0.96756000	-1.73805200	1.36190500
C	-2.52040000	-1.09514300	1.18294400
H	-3.15334500	-1.39911700	2.02382400
H	-2.42446400	-0.00842200	1.19354600
C	-3.12353100	-1.55506800	-0.15870000
H	-2.40092100	-1.30198100	-0.94033400
H	-3.25561600	-2.64312300	-0.14759000
C	-4.44209200	-0.87380500	-0.44120000
C	-5.65975300	-1.43698100	-0.04472600
C	-4.45702300	0.36817400	-1.09050900
C	-6.86627100	-0.78084200	-0.28458900
H	-5.66321200	-2.40401900	0.45107600
C	-5.66186900	1.02425400	-1.33010400
H	-3.51356100	0.80154600	-1.41216900
C	-6.86993200	0.45491500	-0.92784500
H	-7.80119600	-1.23565500	0.02755600
H	-5.65564100	1.98333300	-1.83732700
H	-7.80683200	0.96856800	-1.11778000
C	2.35741800	-1.38291300	1.08918400
H	2.47543000	-0.33580200	1.37150000
H	3.00681500	-1.99053700	1.72711500
C	2.70962700	-1.57326300	-0.39968500
H	2.61107100	-2.63189000	-0.66310500
H	1.97047200	-1.01815700	-0.98659300

C	4.10426900	-1.08795500	-0.71619900
C	5.17544800	-1.97628600	-0.85569400
C	4.35317300	0.28402000	-0.85626300
C	6.46244000	-1.51426400	-1.12904500
H	4.99674000	-3.04344800	-0.75806600
C	5.63728200	0.74782800	-1.12763700
H	3.53017200	0.98349700	-0.74912700
C	6.69723800	-0.14838800	-1.26559500
H	7.27871700	-2.22127600	-1.23913000
H	5.80864200	1.81358400	-1.23513100
H	7.69661600	0.21561300	-1.48047800

Complex 3 (neutral):

Ni	1.55512800	-0.62977000	-0.20158300
Br	0.80493900	-0.76267100	2.02462800
C	1.26535400	1.25569200	-0.28818500
C	1.56606500	3.49030000	-0.13120000
C	0.27771500	3.27782800	-0.48814200
H	2.10730300	4.40412300	0.04365900
H	-0.51984500	3.97276100	-0.68656500
C	2.26306700	-2.67627000	-0.55357800
C	1.06477600	-2.55257900	-1.34630400
C	3.24160600	-1.79238300	-1.05833300
H	2.40093300	-3.37633700	0.25684100
C	1.26211000	-1.51638000	-2.25051000

H	0.16054700	-3.12548800	-1.20681700
C	2.59757000	-0.98996200	-2.03125200
H	4.25526200	-1.68725000	-0.70291000
H	0.55453700	-1.14486400	-2.97702800
H	3.05379500	-0.19921100	-2.60975400
N	0.11117900	1.90385000	-0.58590100
N	2.15759900	2.24030700	-0.01806900
C	-1.16620400	1.23162600	-0.83972900
H	-1.62550900	1.67620300	-1.72696100
H	-0.92790400	0.19271900	-1.06346400
C	-2.11479700	1.30805600	0.37017300
H	-1.57415600	0.92876400	1.24053700
H	-2.37427400	2.35342200	0.56645000
C	-3.36898900	0.49616600	0.13706700
C	-4.50616200	1.06774500	-0.44238800
C	-3.39886300	-0.86212300	0.47438500
C	-5.64656900	0.30390800	-0.68238900
H	-4.50363500	2.12311900	-0.69903100
C	-4.53769500	-1.62746700	0.23565600
H	-2.52545100	-1.31226900	0.93569900
C	-5.66449000	-1.04735800	-0.34452200
H	-6.52165500	0.76501300	-1.12716500
H	-4.54717000	-2.67666300	0.50965300
H	-6.55221300	-1.64271900	-0.52641800
C	3.52460400	2.00779900	0.43153600

H	3.61558600	2.23394300	1.49559800
H	3.75406400	0.95644900	0.27369200
H	4.21730600	2.62862400	-0.13959800

Complex 3 (cation, oxidized):

Ni	1.55587100	-0.63897700	-0.24370800
Br	1.17169700	-0.81415700	2.00008600
C	1.17611500	1.26678400	-0.25813400
C	1.39714900	3.48955400	-0.08380600
C	0.10597700	3.22886800	-0.39795300
H	1.90770700	4.42231000	0.08356400
H	-0.72660300	3.89289800	-0.55333100
C	2.04961500	-2.68259000	-0.78349000
C	0.97384200	-2.25881600	-1.61636000
C	3.18775300	-1.86501900	-1.05984400
H	2.01793800	-3.49917000	-0.07804500
C	1.40712600	-1.12131000	-2.32704000
H	-0.01611700	-2.68950000	-1.63946400
C	2.79194300	-0.87880100	-1.98218500
H	4.15475000	-1.95015100	-0.58701300
H	0.82864700	-0.54741500	-3.03539400
H	3.41031900	-0.09437100	-2.39167700
N	-0.01437400	1.85090800	-0.50282400
N	2.04407300	2.26601000	0.00447800
C	-1.28750200	1.14334500	-0.72769600

H	-1.75940700	1.56824400	-1.61607700
H	-1.04056100	0.10490100	-0.94610600
C	-2.23246800	1.21669700	0.48391400
H	-1.70828400	0.82894500	1.36091900
H	-2.47954500	2.26240600	0.68939900
C	-3.49530800	0.42214700	0.22812700
C	-4.57992900	0.99885500	-0.44049500
C	-3.58633200	-0.91357700	0.63304600
C	-5.72907000	0.25688400	-0.70214300
H	-4.53497800	2.04020600	-0.74509100
C	-4.73535300	-1.65732100	0.37349700
H	-2.76197800	-1.36796000	1.17431200
C	-5.80817500	-1.07383100	-0.29686500
H	-6.56548900	0.71993600	-1.21260100
H	-4.79800000	-2.68732500	0.70528400
H	-6.70514800	-1.64932000	-0.49292100
C	3.45917200	2.09984300	0.33944600
H	3.75353400	2.88590900	1.03305900
H	3.59754600	1.13691800	0.82657400
H	4.07668000	2.16072300	-0.55826700

Complex 3 (anion, reduced):

Ni	-1.61316000	-0.49673300	0.12035300
Br	0.07178200	-1.65421600	-1.45085300
C	-1.08789700	1.41233300	-0.04259900

C	-1.16084000	3.65736000	-0.45069900
C	0.10025700	3.36124200	-0.05529500
H	-1.60712600	4.59649100	-0.73244700
H	0.96127600	3.99500500	0.07586400
C	-3.38477800	-2.09499000	0.28747000
C	-2.62302500	-1.89803500	1.47651700
C	-4.44802700	-1.15956400	0.29143900
H	-3.20946700	-2.86507100	-0.45104900
C	-3.21357500	-0.81550800	2.18992900
H	-1.81572100	-2.52952200	1.82463200
C	-4.34041800	-0.37562600	1.46075000
H	-5.20399200	-1.05849500	-0.47897300
H	-2.87814500	-0.42864400	3.14442500
H	-4.99511900	0.44265600	1.74096500
N	0.12723000	1.99631800	0.19131700
N	-1.86833000	2.46426600	-0.43629700
C	1.30985900	1.25483700	0.62299900
H	1.72793100	1.74276400	1.51047600
H	0.95848300	0.26078000	0.89865500
C	2.37167800	1.13986900	-0.48582600
H	1.90635500	0.60447300	-1.31821500
H	2.65807700	2.14082100	-0.82808600
C	3.59678100	0.39353900	-0.00847800
C	4.73960400	1.07287800	0.42697600
C	3.59419100	-1.00778800	0.02998100

C	5.85666200	0.37842400	0.88975100
H	4.75698400	2.15905000	0.39676400
C	4.70964300	-1.70150000	0.49275500
H	2.70922100	-1.53798500	-0.31443500
C	5.84396400	-1.01394400	0.92465700
H	6.73514400	0.92436700	1.21948800
H	4.69212000	-2.78628800	0.51256800
H	6.71133600	-1.55905200	1.28302300
C	-3.26567200	2.33145700	-0.82059000
H	-3.39666100	2.59460800	-1.87460700
H	-3.56449200	1.29563000	-0.65932900
H	-3.89282800	2.98049000	-0.20331000

Complex 4 (neutral):

Ni	-0.13182400	1.59185200	-0.13411100
Br	0.04772900	0.51697700	1.95626600
C	-0.53253300	-0.02111300	-1.08043900
C	-1.64451500	-1.73259600	-2.05451100
C	-0.32129900	-1.99680200	-2.15571100
H	-2.50413300	-2.29502400	-2.37449800
H	0.19660300	-2.83227700	-2.59412800
C	0.03996700	3.70047600	0.45184400
C	1.29249900	3.38687000	-0.19396300
C	-1.00151200	3.59913500	-0.49331900
H	-0.06558700	4.01575400	1.47916400

C	1.01074100	2.98468600	-1.49262100
H	2.26174700	3.40580200	0.28105900
C	-0.42977000	3.04282200	-1.66554300
H	-2.04557400	3.81350400	-0.32405200
H	1.71862100	2.65808100	-2.24000500
H	-0.95237500	2.82116500	-2.58524200
N	0.34695000	-0.93662400	-1.55814200
N	-1.75575300	-0.51662200	-1.39477000
C	1.79648400	-0.87273300	-1.35138700
H	2.29363700	-1.08877400	-2.30107200
H	2.02444200	0.15571800	-1.07476400
C	2.27276100	-1.83617900	-0.24905400
H	1.68477400	-1.63084600	0.64859500
H	2.07062300	-2.86826500	-0.55332100
C	3.74652700	-1.65737900	0.03797700
C	4.71508900	-2.38764600	-0.65802900
C	4.16793500	-0.72548000	0.99377500
C	6.07228100	-2.19286800	-0.40979000
H	4.40490100	-3.12382300	-1.39395400
C	5.52397300	-0.52958500	1.24395500
H	3.42369900	-0.16203400	1.54779800
C	6.48036900	-1.26132600	0.54217700
H	6.80949200	-2.77224900	-0.95481400
H	5.83344200	0.19093300	1.99299700
H	7.53577700	-1.11108800	0.74002200

C	-3.02737600	0.13911700	-1.05938400
H	-2.75273400	1.05935000	-0.54181000
H	-3.53510700	0.41183800	-1.98870100
C	-3.93270700	-0.72089400	-0.20393600
C	-5.18191500	-1.12238300	-0.68108400
C	-3.53448700	-1.10696400	1.08164900
C	-6.02781300	-1.89909100	0.11033800
H	-5.50062700	-0.82168400	-1.67464500
C	-4.37801700	-1.88454500	1.86843700
H	-2.56721900	-0.79447200	1.46416500
C	-5.62543500	-2.28242800	1.38619800
H	-6.99673800	-2.20198600	-0.27051300
H	-4.06244500	-2.17559300	2.86397400
H	-6.28050700	-2.88594200	2.00447700

Complex 4 (cation, oxidized):

Ni	-0.02899400	1.64556700	-0.15739900
Br	-0.10203200	0.89822000	2.00095200
C	-0.48286500	-0.09487900	-0.89379100
C	-1.63736300	-1.86855700	-1.62610500
C	-0.31994700	-2.16405700	-1.73041000
H	-2.51348300	-2.44868400	-1.85710000
H	0.17476700	-3.05237200	-2.08339900
C	0.52640000	3.73199500	0.09913800
C	1.47781000	3.12752700	-0.77231800

C	-0.75586200	3.68959100	-0.52789700
H	0.74148500	4.16809500	1.06300900
C	0.77562000	2.61999300	-1.88448100
H	2.53375000	3.01514900	-0.57641200
C	-0.61939800	2.97587000	-1.73300500
H	-1.67448400	4.07561600	-0.11183400
H	1.19853200	2.09080000	-2.72507500
H	-1.40315000	2.75163600	-2.44056000
N	0.38217800	-1.05729900	-1.27423700
N	-1.72068500	-0.58681300	-1.10357700
C	1.84709500	-1.00240900	-1.13272700
H	2.29053100	-1.30876900	-2.08256600
H	2.11281500	0.04085600	-0.96464200
C	2.37324900	-1.87361400	0.02107400
H	1.87169500	-1.57315200	0.94449200
H	2.11215300	-2.91942300	-0.16496000
C	3.87316800	-1.72613100	0.16079900
C	4.74427000	-2.53555100	-0.57519300
C	4.41265700	-0.75284600	1.00852300
C	6.12370300	-2.37443500	-0.46959300
H	4.34400100	-3.30886700	-1.22396800
C	5.79190200	-0.59002300	1.11600200
H	3.74930000	-0.13384800	1.60517200
C	6.65025200	-1.39942800	0.37491400
H	6.78667500	-3.01566000	-1.03874500

H	6.19660200	0.15886400	1.78709000
H	7.72349600	-1.27853200	0.46291600
C	-2.98852200	0.13365200	-0.83687100
H	-2.72586700	0.97920800	-0.20001700
H	-3.36283000	0.52363200	-1.78646600
C	-4.03334800	-0.73527700	-0.17880600
C	-5.18250000	-1.10476100	-0.88140400
C	-3.86769500	-1.16515000	1.14290800
C	-6.15561300	-1.89710100	-0.27404200
H	-5.32551700	-0.76646800	-1.90287500
C	-4.83772200	-1.95768800	1.74674200
H	-2.98194000	-0.87637100	1.69911000
C	-5.98274300	-2.32495400	1.03905300
H	-7.04633300	-2.17483300	-0.82490400
H	-4.70572700	-2.28359500	2.77169600
H	-6.73926300	-2.93866500	1.51354400

Complex 4 (anion, reduced):

Ni	-0.41059400	1.47795700	-0.18418700
Br	0.51495000	0.43459300	2.02995500
C	-0.49483600	-0.18248000	-1.26577800
C	-1.29641200	-2.04256100	-2.32065600
C	0.05557000	-2.11175600	-2.35232900
H	-2.04526700	-2.71931500	-2.69607000
H	0.70961500	-2.85513300	-2.77625200

C	-1.20978800	3.50897200	0.58904000
C	-0.16766000	3.68249000	-0.36726300
C	-2.42004300	3.29012700	-0.11791500
H	-1.10047500	3.58177800	1.66181900
C	-0.74216400	3.54020600	-1.66055300
H	0.85732100	3.95117100	-0.14804200
C	-2.12964400	3.30954700	-1.49978200
H	-3.39263100	3.12683200	0.32996200
H	-0.21416600	3.62620400	-2.60202800
H	-2.84098400	3.15057600	-2.30249400
N	0.52590000	-0.97349300	-1.71108600
N	-1.61331500	-0.86145800	-1.66409600
C	1.93200400	-0.67207900	-1.45823700
H	2.48561300	-0.72591900	-2.40221500
H	1.95289900	0.35718800	-1.09892700
C	2.55226900	-1.60754900	-0.40392800
H	1.93745100	-1.52660600	0.49712700
H	2.51466700	-2.64285200	-0.76147400
C	3.97940300	-1.22257700	-0.08944900
C	5.06083700	-1.82934400	-0.73689200
C	4.23916000	-0.21716700	0.85204500
C	6.37215800	-1.44727300	-0.45675300
H	4.87330000	-2.61560400	-1.46317300
C	5.54877200	0.16511900	1.13183800
H	3.40051800	0.24781700	1.36434600

C	6.61965800	-0.44603100	0.47955400
H	7.19824500	-1.93307700	-0.96663800
H	5.73250600	0.94230400	1.86636500
H	7.63876900	-0.14625300	0.70165100
C	-2.97066500	-0.42544800	-1.33588600
H	-2.88913200	0.63481900	-1.08123400
H	-3.59230100	-0.51432300	-2.23193800
C	-3.58616800	-1.20602500	-0.19103900
C	-4.76991800	-1.92481400	-0.36996300
C	-2.98045700	-1.19124900	1.07211500
C	-5.34800700	-2.62330000	0.69055700
H	-5.24774000	-1.93491700	-1.34582900
C	-3.55596700	-1.89179700	2.12750500
H	-2.06059400	-0.63378300	1.23199900
C	-4.73915800	-2.60868600	1.94249100
H	-6.26876500	-3.17699800	0.53661800
H	-3.07356500	-1.86939700	3.09850400
H	-5.18364400	-3.15134100	2.77067300

Complex 5 (neutral):

Br	0.00028700	0.83455400	2.09159700
Ni	0.00022000	1.88736400	-0.01590900
N	-1.07482000	-0.49568600	-1.36286000
C	-3.28649600	-1.17723100	-0.44627100
C	-2.99066800	-1.55557500	0.86883100

C	-2.47282500	-0.10171900	-1.13198300
C	-3.74755000	-2.53803400	1.49880600
C	-4.34856100	-1.79322000	-1.11144700
C	-4.80662700	-3.15108300	0.82819800
C	-5.10809300	-2.77643200	-0.47774300
C	-0.00002200	0.23177200	-0.96913500
C	-0.67653200	-1.66668700	-1.99388600
C	0.00025800	3.23864800	-1.64429500
C	-1.16675500	3.59129500	-0.88381200
C	-0.72302100	3.97668100	0.38166900
H	0.00017300	2.90551400	-2.67259300
H	-2.42467900	0.80334700	-0.52560800
H	-4.58913700	-1.49949300	-2.12880200
H	-2.92567800	0.15740400	-2.09321300
H	-5.93201100	-3.24561500	-1.00371600
H	-3.51384400	-2.82193400	2.51871900
H	-2.19111800	3.50363900	-1.21238200
H	-1.38254200	-2.39383200	-2.35475400
H	-2.17097500	-1.07404300	1.39357400
H	-1.34182300	4.23267300	1.22874300
H	-5.39533800	-3.91468300	1.32417500
N	1.07458200	-0.49588900	-1.36300300
C	3.28615300	-1.17777300	-0.44646300
C	2.99028400	-1.55589600	0.86869400
C	2.47268100	-0.10218000	-1.13227400

C	3.74698100	-2.53843400	1.49876700
C	4.34807200	-1.79406000	-1.11159500
C	4.80591400	-3.15178000	0.82820300
C	5.10742100	-2.77734900	-0.47779300
C	0.67599600	-1.66683900	-1.99393100
H	2.42474200	0.80295700	-0.52598700
H	4.58867900	-1.50050600	-2.12899300
H	2.92553800	0.15675800	-2.09355400
H	5.93122800	-3.24676500	-1.00373200
H	3.51324300	-2.82216700	2.51872000
H	1.38182000	-2.39413800	-2.35485600
H	2.17069800	-1.07413900	1.39339900
H	5.39448000	-3.91544200	1.32425500
C	1.16741500	3.59107200	-0.88393300
C	0.72388300	3.97654000	0.38159600
H	2.19172900	3.50322100	-1.21260700
H	1.34282100	4.23241100	1.22860600

Complex 5 (cation, oxidized):

Br	0.01685500	1.10708400	2.10307800
Ni	0.01536600	1.95515400	-0.01934500
N	-1.08743800	-0.54112800	-1.14771100
C	-3.36298400	-1.21395900	-0.37373700
C	-3.17864600	-1.65232400	0.94268000
C	-2.49322400	-0.11934200	-0.94405300

C	-3.99100100	-2.65188500	1.46666200
C	-4.37131300	-1.78639300	-1.15232600
C	-4.99615000	-3.22049200	0.68357900
C	-5.18691200	-2.78666100	-0.62508700
C	0.00023300	0.19182400	-0.83532600
C	-0.69629900	-1.75757800	-1.68789800
C	0.74867000	3.17808000	-1.62056400
C	-0.69859500	3.18229200	-1.62502100
C	-1.13498500	3.78662800	-0.42977200
H	1.37601500	2.80618900	-2.41648300
H	-2.45447700	0.73814500	-0.27089500
H	-4.52898700	-1.44587300	-2.17089100
H	-2.88988100	0.21735200	-1.90490600
H	-5.96981900	-3.22165700	-1.23483500
H	-3.84606800	-2.98373100	2.48797000
H	-1.32301500	2.81397700	-2.42489000
H	-1.41035200	-2.50461600	-1.98703500
H	-2.40225200	-1.20849300	1.55709500
H	-2.15960000	3.92421900	-0.11812800
H	-5.63044300	-3.99627800	1.09582000
N	1.07323500	-0.55522600	-1.16438000
C	3.34219200	-1.25217400	-0.39266000
C	3.15376600	-1.66460900	0.93154300
C	2.48771000	-0.15480800	-0.98095000
C	3.95268800	-2.66626400	1.47181900

C	4.34074300	-1.85278300	-1.16255500
C	4.94829300	-3.26299100	0.69747300
C	5.14286900	-2.85519900	-0.61894900
C	0.65783300	-1.76649600	-1.69810800
H	2.47013400	0.71848400	-0.32759600
H	4.50143200	-1.53270300	-2.18727100
H	2.88259300	0.15284300	-1.95219800
H	5.91826300	-3.31215300	-1.22220300
H	3.80470100	-2.97803700	2.49900400
H	1.35738700	-2.52305700	-2.00746100
H	2.38455800	-1.19941200	1.53920100
H	5.57213300	-4.04038200	1.12243600
C	1.18090100	3.77903800	-0.42244300
C	0.02137500	4.09940900	0.34410000
H	2.20426300	3.90987900	-0.10381600
H	0.01968000	4.52762700	1.33519000

Complex 5 (anion, reduced):

Br	-0.00087500	0.46621600	2.33381400
Ni	0.00549000	1.79620500	0.07233000
N	-1.07187400	-0.48436000	-1.59727600
C	-3.24375600	-1.12774500	-0.56860700
C	-2.87210700	-1.46924600	0.73853100
C	-2.45537200	-0.08763200	-1.33623500
C	-3.60789600	-2.41721900	1.44318100

C	-4.35651900	-1.74556000	-1.14435600
C	-4.71740300	-3.03342600	0.86188600
C	-5.09326700	-2.69462400	-0.43498600
C	0.00044200	0.21866700	-1.12616300
C	-0.68219900	-1.59840400	-2.32946100
C	0.02511700	3.89397300	-1.59610200
C	-1.13075100	3.90435000	-0.77937000
C	-0.70735300	3.90555900	0.57656000
H	0.03537000	3.85956800	-2.67917000
H	-2.37661500	0.84659700	-0.77327200
H	-4.65256500	-1.47896100	-2.15526100
H	-2.94965300	0.12948600	-2.28902900
H	-5.95594700	-3.16569500	-0.89530200
H	-3.31275800	-2.66806400	2.45643700
H	-2.15717600	3.91995600	-1.12445800
H	-1.38802200	-2.28974700	-2.75759100
H	-2.01418700	-0.98552500	1.20498600
H	-1.34700800	3.94181400	1.44756600
H	-5.28678300	-3.77072000	1.41886700
N	1.06825500	-0.48979800	-1.59938800
C	3.23702500	-1.14282300	-0.57010800
C	2.86347700	-1.47865100	0.73795400
C	2.45427100	-0.10053600	-1.34059200
C	3.59422100	-2.42847200	1.44536000
C	4.34653200	-1.76811700	-1.14403600

C	4.70052200	-3.05212500	0.86590900
C	5.07823400	-2.71901200	-0.43190400
C	0.67147400	-1.60187900	-2.33074400
H	2.38158900	0.83592400	-0.78049200
H	4.64406100	-1.50594200	-2.15566300
H	2.94909300	0.11059500	-2.29444100
H	5.93843800	-3.19595400	-0.89080600
H	3.29762100	-2.67487200	2.45927700
H	1.37290700	-2.29683100	-2.76025700
H	2.00799100	-0.98930500	1.20301600
H	5.26599100	-3.79080800	1.42503200
C	1.16514100	3.89751900	-0.75737300
C	0.71568000	3.90124100	0.59027000
H	2.19811000	3.90773600	-1.08254700
H	1.33870900	3.93352600	1.47335400

Complex 6 (neutral):

Br	1.28734900	-1.65207400	-1.37786800
N	0.11552400	1.71673900	0.18340600
C	-2.00997200	0.65965700	0.91854600
C	-2.15735900	-0.33562300	-0.05661400
C	-0.62996600	1.14659100	1.30865800
C	-3.42209500	-0.79161300	-0.40454400
C	-3.14369400	1.18638300	1.54314400
C	-4.53313400	-0.24603000	0.23180300

C	-4.41611900	0.73682000	1.20553800
C	1.29363800	1.22350500	-0.27819400
C	-0.29852000	2.80556300	-0.57316600
C	3.12478800	0.35171600	2.13876600
C	2.68953600	-0.97228900	2.38779600
C	3.37153200	-1.79986600	1.46879300
H	2.79591300	1.24003600	2.65922100
H	-0.01887800	0.32112200	1.67779900
H	-3.03575200	1.95336900	2.30269900
H	-0.70408800	1.89568600	2.10136400
H	-5.30605900	1.13140800	1.67511500
H	-3.55943100	-1.56059200	-1.15182000
H	1.92119000	-1.27997800	3.08048000
H	-1.21510600	3.33331600	-0.37543300
H	-1.28068200	-0.75662700	-0.54089900
H	3.22012400	-2.86112600	1.33955400
N	1.61765400	2.02443100	-1.32129900
C	0.64705800	2.99539700	-1.52202900
H	0.71501400	3.72516300	-2.31031000
C	4.21854800	0.30485900	1.18402400
C	4.36903700	-1.01632300	0.78194600
H	4.79010500	1.15705400	0.84680900
H	5.05788300	-1.39347300	0.04122200
C	2.75306200	1.78867000	-2.20768600
H	3.14122900	2.74373600	-2.56341600

H	3.52242200	1.26157200	-1.64833500
H	2.44682500	1.16707300	-3.05041300
N	-5.88419500	-0.72570700	-0.13872200
O	-5.96134400	-1.59311400	-0.99695900
O	-6.84056500	-0.22276000	0.43636300
Ni	2.24237200	-0.32360400	0.31436200

Complex 6 (cation, oxidized):

Br	1.50441300	-1.70970000	-1.29895100
N	0.03460200	1.50738800	0.16351300
C	-2.10482600	0.44790100	0.87808000
C	-2.34587900	-0.47765600	-0.14471300
C	-0.68711300	0.81899900	1.25361300
C	-3.64634700	-0.82957000	-0.48047200
C	-3.18056400	1.01455800	1.56599500
C	-4.69698700	-0.24668500	0.21949600
C	-4.48936400	0.66888200	1.24043900
C	1.25764200	1.17626800	-0.30075700
C	-0.46364100	2.59488000	-0.53963900
C	2.97178700	0.29491600	2.24761600
C	2.91592300	-1.11219000	2.24971400
C	3.82991900	-1.58272800	1.26046000
H	2.39696700	0.96282900	2.87135900
H	-0.10476800	-0.07197400	1.49114600
H	-3.00312100	1.72568600	2.36546200

H	-0.68507300	1.46966600	2.13083300
H	-5.33852400	1.09265500	1.75834500
H	-3.86108000	-1.54368400	-1.26327700
H	2.25357400	-1.72747400	2.84031700
H	-1.43284200	3.01530400	-0.33603900
H	-1.51609400	-0.92676900	-0.67917900
H	3.98522000	-2.61536400	0.98613900
N	1.53087400	2.04501000	-1.29646600
C	0.47492900	2.93032400	-1.45552900
H	0.48505300	3.70710600	-2.20052200
C	3.98035300	0.70076900	1.29117800
C	4.52870100	-0.46261100	0.71844300
H	4.27678900	1.71946500	1.09105200
H	5.28975600	-0.50395900	-0.04640600
C	2.72231200	2.00844400	-2.14861900
H	2.64430900	2.80139400	-2.88919700
H	3.62077500	2.17108400	-1.55378300
H	2.78245900	1.04724200	-2.65844800
N	-6.09197600	-0.61937000	-0.13836100
O	-6.23712500	-1.43409000	-1.03540600
O	-6.99014600	-0.08249600	0.48936700
Ni	2.38052700	-0.30532900	0.27468500

Complex 6 (anion, reduced):

Br	1.13790000	-1.85882700	-1.41556300

N	0.08793100	1.83167000	0.00292100
C	-2.00263700	0.80854600	0.86895800
C	-2.15069100	-0.27145700	-0.01799900
C	-0.63189000	1.35545400	1.18242900
C	-3.41012100	-0.78570400	-0.28795000
C	-3.13995700	1.35072900	1.48021600
C	-4.53146900	-0.22239100	0.32933100
C	-4.40622400	0.84482800	1.21943900
C	1.28094100	1.29824700	-0.38780400
C	-0.34581300	2.82263500	-0.86852000
C	3.29028100	0.28829300	2.49150800
C	2.90349500	-1.07756900	2.39027200
C	3.69452000	-1.67851700	1.37443200
H	2.87467200	1.01638700	3.17626000
H	0.01715100	0.57580000	1.60160700
H	-3.03155900	2.18165800	2.17070900
H	-0.70780600	2.16661900	1.91367400
H	-5.29420400	1.25415200	1.67975200
H	-3.54107200	-1.61861500	-0.96439600
H	2.17107500	-1.58178500	3.00606700
H	-1.27508300	3.35026500	-0.73846700
H	-1.27459600	-0.71255900	-0.49109000
H	3.64427600	-2.70996800	1.05814100
N	1.58728600	1.99610300	-1.51464300
C	0.60242800	2.92114900	-1.83099400

H	0.65763500	3.55712900	-2.69851600
C	4.32131400	0.52297900	1.55239400
C	4.56909600	-0.68614300	0.85683900
H	4.81173700	1.47150800	1.37332100
H	5.30362200	-0.83633100	0.07678800
C	2.72593300	1.65760500	-2.35655600
H	3.13236100	2.56306900	-2.81371100
H	3.47713400	1.18554400	-1.72565800
H	2.42566100	0.94316900	-3.12591700
N	-5.85737800	-0.75258800	0.04202400
O	-5.95113400	-1.69418500	-0.75211400
O	-6.82817000	-0.23140400	0.60762400
Ni	2.20274300	-0.31288500	0.33978500

Complex 7 (neutral):

Br	0.68272200	-0.68965000	2.08144100
Ni	1.35277700	-1.84697800	0.14039700
N	1.58452000	0.66978600	-1.36646700
C	3.16043200	2.30242800	-0.34401600
C	2.53161800	2.67208000	0.85083500
C	2.96354700	0.91432400	-0.91097100
C	2.71957600	3.94794500	1.37227500
C	3.97934100	3.22472100	-0.99881900
C	3.53730200	4.86585300	0.71205800
C	4.16937200	4.50257300	-0.47344800

C	0.84908300	-0.41502200	-1.02184700
C	0.86357900	1.51603900	-2.19817400
C	1.86012000	-3.35830400	-1.26830200
C	3.13153900	-2.94241500	-0.70558400
C	3.09984600	-3.22835600	0.65266600
H	1.59610000	-3.29568600	-2.31450600
H	3.16423700	0.14810400	-0.16178700
H	4.47749400	2.94208500	-1.92133900
H	3.64105300	0.75136800	-1.75371000
H	4.81004200	5.20914400	-0.98894000
H	2.23208600	4.22482700	2.30017200
H	3.93419200	-2.46945400	-1.25153600
H	1.26642800	2.44484000	-2.56209100
H	1.90299700	1.95371000	1.36787000
H	3.86171600	-2.99504900	1.38112600
N	-0.34192200	-0.23870200	-1.64989500
C	-2.72147900	-0.52676200	-0.98430700
C	-2.70874000	0.02960800	0.30145400
C	-1.47151100	-1.16691100	-1.55129900
C	-3.86016800	0.59926800	0.82862200
C	-3.90226700	-0.50833400	-1.73154100
C	-5.02074700	0.60515000	0.06040200
C	-5.06348900	0.05685100	-1.21452100
C	-0.34951300	0.94580800	-2.37678300
H	-1.12961200	-1.98139000	-0.91015400

H	-3.91996200	-0.94177100	-2.72582000
H	-1.67695100	-1.57962200	-2.54261500
H	-5.98704800	0.08182600	-1.77540700
H	-3.87449600	1.03005400	1.81998900
H	-1.21042800	1.27961800	-2.92932700
H	-1.79760900	0.00674500	0.89216300
C	1.11167000	-4.01356700	-0.25599800
C	1.82126900	-3.83217600	0.94778400
H	0.14511600	-4.48032300	-0.36851600
H	1.49466800	-4.14140900	1.92942400
N	-6.25050000	1.21370500	0.61698200
O	-7.25478100	1.20159600	-0.08267600
O	-6.18688400	1.69202600	1.74049300
H	3.68331900	5.85820300	1.12365100

Complex 7 (cation, oxidized):

Br	0.81200300	-0.98624200	2.10790100
Ni	1.48713200	-1.87599600	0.11365100
N	1.53029800	0.76458300	-1.21052000
C	3.14287300	2.44002600	-0.30659400
C	2.59070000	2.83051300	0.91892400
C	2.93631300	1.03743900	-0.82585900
C	2.79171100	4.12093500	1.39634000
C	3.90077500	3.35491600	-1.04090600
C	3.54862500	5.03103000	0.65752600

C	4.10433100	4.64738100	-0.55948800
C	0.83942800	-0.35309800	-0.91047100
C	0.73049700	1.63590000	-1.93563900
C	1.60862100	-3.40550300	-1.38445600
C	2.89224700	-2.74991500	-1.24825200
C	3.37457800	-3.00443700	0.05030900
H	1.00474600	-3.41845100	-2.27926200
H	3.18938800	0.29744100	-0.06555100
H	4.34231100	3.05786000	-1.98700300
H	3.56700200	0.85960600	-1.70008000
H	4.69768600	5.34947000	-1.13298400
H	2.36513300	4.41635400	2.34757100
H	3.39686100	-2.19533700	-2.02487800
H	1.08420400	2.59887500	-2.26003000
H	2.00664700	2.12367300	1.49930900
H	4.29797200	-2.63905400	0.47435800
N	-0.39486700	-0.18901800	-1.43263900
C	-2.79426800	-0.53037000	-0.84583900
C	-2.86874400	0.03089900	0.43480100
C	-1.50575400	-1.15602500	-1.33331100
C	-4.05694100	0.58663300	0.88977800
C	-3.92484100	-0.53213700	-1.66629300
C	-5.16529700	0.57163300	0.05016100
C	-5.12318200	0.01947000	-1.22149100
C	-0.47604500	1.03876000	-2.07579200

H	-1.17262400	-1.93463200	-0.64593000
H	-3.87865300	-0.97031400	-2.65734300
H	-1.65492000	-1.61158000	-2.31489300
H	-6.01193400	0.02890500	-1.83699400
H	-4.14275300	1.02274500	1.87532400
H	-1.38025000	1.37891200	-2.54961700
H	-1.99729100	0.03018000	1.07989900
C	1.31998500	-4.05197500	-0.16726800
C	2.37811100	-3.75440500	0.74263500
H	0.42784200	-4.61444200	0.06466000
H	2.42713700	-4.06551800	1.77534900
N	-6.43982000	1.16705200	0.53243600
O	-7.39140300	1.14021500	-0.23118500
O	-6.44203800	1.64137100	1.65715800
H	3.70761400	6.03463800	1.03374600

Complex 7 (anion, reduced):

Br	0.52127400	-0.48856100	2.24504400
Ni	1.45982800	-1.71570200	0.17563000
N	1.51292800	0.74025000	-1.62937400
C	3.05568500	2.34934900	-0.52195200
C	2.45948100	2.50168300	0.73664100
C	2.90122400	1.05036600	-1.28549100
C	2.61807000	3.69201100	1.43971900
C	3.80670800	3.40039100	-1.05273100

C	3.36949500	4.73925900	0.90421500
C	3.96632800	4.59177700	-0.34471100
C	0.85573000	-0.35063100	-1.14432000
C	0.69828300	1.51362000	-2.44733800
C	3.31760000	-3.03872100	-1.00211600
C	3.63185700	-2.82618400	0.36345200
C	2.60804800	-3.42320400	1.14644900
H	3.89452100	-2.68889500	-1.84900700
H	3.24304700	0.19977500	-0.69088200
H	4.27545400	3.28559100	-2.02610200
H	3.49520600	1.08204400	-2.20451100
H	4.55353100	5.39959700	-0.76919200
H	2.15424700	3.79583500	2.41458900
H	4.50515000	-2.31557900	0.74707200
H	1.03189300	2.43193100	-2.89969500
H	1.87733200	1.68835100	1.16692600
H	2.56044000	-3.44028300	2.22532500
N	-0.38851000	-0.23872700	-1.69183500
C	-2.72133000	-0.64630200	-0.93831300
C	-2.75248700	-0.00116400	0.30895400
C	-1.43470900	-1.23452800	-1.46148200
C	-3.94016100	0.52652700	0.79365800
C	-3.90487900	-0.75818000	-1.67885900
C	-5.10589700	0.40926400	0.03121600
C	-5.10078400	-0.23557400	-1.20495100

C	-0.50415400	0.89314600	-2.48940900
H	-0.99318300	-1.93420200	-0.74083100
H	-3.88910100	-1.26284800	-2.63992700
H	-1.62257800	-1.77916600	-2.39255600
H	-6.02196700	-0.31065600	-1.76510800
H	-3.98341700	1.02063300	1.75413200
H	-1.41863500	1.16480900	-2.98827000
H	-1.84261400	0.06536900	0.90333000
C	2.10171200	-3.75896000	-1.06903500
C	1.66146500	-4.00499300	0.26097800
H	1.59713600	-4.07373400	-1.97338800
H	0.78587700	-4.57008500	0.55044900
N	-6.35712100	0.96928100	0.53235000
O	-7.37013800	0.84558300	-0.16569000
O	-6.34315100	1.54035300	1.62553600
H	3.48942000	5.66394900	1.45926500

Complex 8 (neutral):

Ni	-0.80074100	1.75483700	-0.14361200
Br	-0.47723200	0.21551600	-1.89953900
C	-0.24996200	0.51457500	1.20559800
C	1.01117400	-0.66678500	2.66865200
C	-0.24359500	-1.17068200	2.71099800
H	1.90381700	-0.95015900	3.19855200
H	-0.65717900	-1.97505200	3.29444000

C	-1.30717100	3.56664800	-1.26010900
C	-2.53632700	3.16308300	-0.62178700
C	-0.36931600	3.92704900	-0.26730900
H	-1.15699400	3.63743800	-2.32705800
C	-2.31578700	3.15470300	0.74931900
H	-3.43770900	2.86189800	-1.13364600
C	-0.94102700	3.56721700	0.97637500
H	0.62404600	4.31454000	-0.43390400
H	-3.02030800	2.87693900	1.51927800
H	-0.48681400	3.69531100	1.94867100
N	-1.00409900	-0.43365000	1.81342900
N	0.98974400	0.36664400	1.74074000
C	-2.40345400	-0.71447100	1.47532000
H	-2.97374000	-0.80384200	2.40391600
H	-2.76924700	0.15705800	0.93438100
C	-2.55598400	-1.97906400	0.61100600
H	-1.89925300	-1.87171700	-0.25544300
H	-2.22158000	-2.85346600	1.17835200
C	-3.98772000	-2.16698100	0.16142500
C	-4.88995100	-2.92904800	0.91009900
C	-4.44144200	-1.54952100	-1.01012400
C	-6.21499700	-3.07086100	0.50260000
H	-4.55076500	-3.42559900	1.81450400
C	-5.76524200	-1.68963900	-1.41908700
H	-3.74506400	-0.96802500	-1.60600100

C	-6.65648400	-2.44940600	-0.66320500
H	-6.89970500	-3.67110000	1.09162100
H	-6.09887000	-1.21136800	-2.33333700
H	-7.68592200	-2.56189500	-0.98427200
C	2.14945800	1.18352900	1.37311300
H	1.78008800	1.91171400	0.64888800
H	2.49195800	1.72820900	2.25687100
C	3.28741900	0.37368800	0.78690400
C	4.54264100	0.38048900	1.40132100
C	3.09697900	-0.36713600	-0.38689200
C	5.60349500	-0.34006600	0.86238200
H	4.69812600	0.95660200	2.30725900
C	4.14674100	-1.09327800	-0.93393500
H	2.12795000	-0.36824100	-0.87719900
C	5.38495400	-1.06901500	-0.29890000
H	6.58199900	-0.34797800	1.32138900
H	4.02362500	-1.66891200	-1.84061400
N	6.50711400	-1.84289800	-0.87746900
O	6.28951300	-2.47724200	-1.89979800
O	7.58294800	-1.80046900	-0.29534300

Complex 8 (cation, oxidized):

Ni	0.92803600	1.81232300	0.05667400
Br	0.49769100	0.70139900	2.00700400
C	0.25969600	0.35638300	-1.04818400

C	-1.09098000	-0.99610700	-2.22025000
C	0.15745400	-1.51716500	-2.26992300
H	-2.01808400	-1.34272100	-2.64227700
H	0.52841900	-2.40439400	-2.75329500
C	1.74274800	3.69004000	0.78103900
C	2.72603800	3.07703500	-0.05151700
C	0.59495100	3.98500100	-0.01345900
H	1.85697300	3.91499400	1.83079600
C	2.15563400	2.89903400	-1.32652800
H	3.70335600	2.74425500	0.26496900
C	0.82367300	3.46584500	-1.30259600
H	-0.31005800	4.45884600	0.33636900
H	2.62965000	2.45057600	-2.18659800
H	0.14785500	3.50944900	-2.14332700
N	0.98067800	-0.67056600	-1.54073600
N	-1.01212000	0.16041500	-1.45711700
C	2.40585300	-0.92843000	-1.26638800
H	2.91233200	-1.08526400	-2.22116600
H	2.81174900	-0.02187400	-0.81888100
C	2.62948500	-2.12473500	-0.32536400
H	2.06038500	-1.96031600	0.59298500
H	2.23850900	-3.03375500	-0.79191100
C	4.10129700	-2.28978000	-0.01217900
C	4.93952600	-3.00656900	-0.87219400
C	4.65298800	-1.70078400	1.13033300

C	6.29976400	-3.12900000	-0.59941000
H	4.52571500	-3.48794000	-1.75327500
C	6.01310400	-1.82333800	1.40588800
H	4.01092900	-1.16125500	1.82000000
C	6.83971300	-2.53552500	0.53973300
H	6.93524500	-3.69584700	-1.26978400
H	6.42463400	-1.37400100	2.30236200
H	7.89644800	-2.63729500	0.75677200
C	-2.15669900	1.04348600	-1.15512500
H	-1.80927500	1.74629500	-0.39674400
H	-2.40308300	1.60989300	-2.05614900
C	-3.37138900	0.28791000	-0.66322700
C	-4.56203500	0.32916800	-1.39262800
C	-3.31785600	-0.43437000	0.53522800
C	-5.69397100	-0.34211200	-0.93832600
H	-4.61515100	0.89169600	-2.31840800
C	-4.43825000	-1.11162800	0.99752500
H	-2.39956100	-0.46466200	1.11093600
C	-5.60900500	-1.05323500	0.24941600
H	-6.62740600	-0.32343400	-1.48345500
H	-4.42474400	-1.67438700	1.92057300
N	-6.81185200	-1.77737400	0.74022100
O	-6.70117600	-2.39363600	1.78792700
O	-7.82212600	-1.70473000	0.05954200

Complex 8 (anion, reduced):

Ni	0.72876700	1.70982600	0.23933100
Br	0.56336200	-0.21563700	1.97174200
C	0.24451200	0.59604000	-1.33925900
C	-0.98931600	-0.47409000	-2.93352200
C	0.26943800	-0.97091600	-2.99219600
H	-1.86988600	-0.71758700	-3.50313300
H	0.69534700	-1.72502800	-3.63247700
C	1.47495900	3.40311000	1.54441900
C	2.48948400	3.32931400	0.55152500
C	0.29233000	3.89167500	0.92723400
H	1.58540000	3.14408100	2.58713500
C	1.93342600	3.77054500	-0.67486800
H	3.51060200	3.01042100	0.71192800
C	0.57965700	4.11384600	-0.44772400
H	-0.64528800	4.09684400	1.42605700
H	2.44749300	3.81214100	-1.62665200
H	-0.11452700	4.48935200	-1.18895100
N	1.00597100	-0.30433100	-2.02188600
N	-0.98337900	0.48038800	-1.92422900
C	2.38975900	-0.59803400	-1.65569800
H	3.00084300	-0.63164400	-2.56381000
H	2.72028200	0.24469300	-1.04768400
C	2.51314200	-1.90849700	-0.85523800

H	1.80698600	-1.84639000	-0.02178400
H	2.22559100	-2.75465400	-1.48939500
C	3.91425500	-2.10729200	-0.32559800
C	4.87667200	-2.82311600	-1.04532600
C	4.27843400	-1.54315100	0.90432200
C	6.17352500	-2.97316800	-0.55609000
H	4.60498900	-3.27477400	-1.99552200
C	5.57372400	-1.69216700	1.39359600
H	3.52926800	-0.99976900	1.47340100
C	6.52615700	-2.40548900	0.66616200
H	6.90540400	-3.53595000	-1.12682900
H	5.83743600	-1.25293000	2.34986200
H	7.53392800	-2.52181700	1.05126200
C	-2.13736600	1.25864900	-1.48079800
H	-1.72911900	1.96673700	-0.74888400
H	-2.53399900	1.82920900	-2.32617900
C	-3.22885400	0.41734000	-0.86277800
C	-4.52198600	0.42867800	-1.39880800
C	-2.96533100	-0.36036500	0.27674100
C	-5.54250900	-0.32045700	-0.82805300
H	-4.73308600	1.03394400	-2.27502100
C	-3.97583900	-1.11384100	0.85674500
H	-1.96933300	-0.37001200	0.71608300
C	-5.25577300	-1.09095900	0.29759300
H	-6.54523800	-0.32572200	-1.23109700

H	-3.79041500	-1.71393400	1.73653800
N	-6.32271600	-1.88806600	0.90015900
O	-6.05234400	-2.56781600	1.89155800
O	-7.44390100	-1.84055100	0.38348300

Complex 9 (neutral):

Br	-0.00016900	1.02978400	-2.05546600
Ni	-0.00012900	2.56572200	-0.26784800
N	1.07404300	0.57232700	1.61070200
C	3.27708900	-0.27953600	0.82693300
C	2.94354100	-0.92930600	-0.36870100
C	2.46859600	0.90932100	1.30067700
C	3.69691900	-2.00788900	-0.81319100
C	4.37659000	-0.72178200	1.56756900
C	4.78466300	-2.42715000	-0.05316200
C	5.14118900	-1.79967600	1.13280700
C	-0.00001700	1.18766600	1.05503800
C	0.67605200	-0.41696700	2.50165300
C	-0.00015200	4.27319800	0.97857900
C	1.16737100	4.42564300	0.15456800
C	0.72362700	4.48416800	-1.16695400
H	-0.00012400	4.20796900	2.05753300
H	2.42135200	1.67876700	0.52871200
H	4.64521100	-0.21874200	2.49033500
H	2.92947500	1.34845000	2.18951200

H	5.99596900	-2.15741300	1.68924300
H	3.46091700	-2.52106300	-1.73492800
H	2.19166300	4.42721300	0.49517100
H	1.37975000	-1.03452200	3.03197700
H	2.09793800	-0.58113700	-0.95425300
H	1.34201200	4.52361100	-2.05119700
N	-1.07399100	0.57226400	1.61079300
C	-3.27699600	-0.27972200	0.82707300
C	-2.94343300	-0.92938700	-0.36861300
C	-2.46858200	0.90917000	1.30085700
C	-3.69673700	-2.00800200	-0.81315100
C	-4.37643700	-0.72210500	1.56771600
C	-4.78442400	-2.42740400	-0.05311600
C	-5.14096000	-1.80003300	1.13290600
C	-0.67587100	-0.41697800	2.50174300
H	-2.42142300	1.67865100	0.52891900
H	-4.64506900	-0.21914600	2.49052200
H	-2.92945700	1.34823100	2.18972800
H	-5.99569100	-2.15787700	1.68934700
H	-3.46072300	-2.52109400	-1.73493100
H	-1.37949000	-1.03455100	3.03215200
H	-2.09787600	-0.58111000	-0.95416800
C	-1.16771800	4.42556700	0.15462200
C	-0.72403500	4.48411400	-1.16692100
H	-2.19199700	4.42707000	0.49526900

H	-1.34246300	4.52351400	-2.05113600
N	5.59144900	-3.57760500	-0.52243000
N	-5.59113200	-3.57789400	-0.52243500
O	-6.54256400	-3.91954400	0.16713000
O	-5.25543100	-4.11453500	-1.56821600
O	5.25573200	-4.11436000	-1.56815000
O	6.54292600	-3.91913300	0.16713700

Complex 9 (cation, oxidized):

Br	-0.00073000	1.45104500	2.13210900
Ni	0.00016400	2.69159200	0.21259800
N	-1.07955200	0.45185300	-1.39446300
C	-3.32940800	-0.37687000	-0.71156300
C	-3.08317300	-1.02819500	0.50342400
C	-2.48866500	0.81003200	-1.12531800
C	-3.86334400	-2.10920000	0.89148100
C	-4.37088900	-0.81596600	-1.53256100
C	-4.89047300	-2.52569700	0.05184500
C	-5.16232200	-1.89709600	-1.15421400
C	0.00007000	1.11566000	-0.93105100
C	-0.67648900	-0.63083400	-2.16441200
C	0.00125100	4.71754500	0.99142700
C	1.15900900	4.56079900	0.17226800
C	0.72347600	4.20822200	-1.11955100
H	0.00205400	4.94194900	2.04751800

H	-2.46834900	1.56010500	-0.33393000
H	-4.57574500	-0.31164900	-2.47064900
H	-2.90281400	1.27279200	-2.02394200
H	-5.97519700	-2.25475700	-1.77083500
H	-3.69744900	-2.62769300	1.82559300
H	2.18321100	4.63395700	0.50651400
H	-1.38078900	-1.30574200	-2.61861600
H	-2.28242400	-0.68784400	1.15062000
H	1.34798300	4.00684400	-1.97680000
N	1.07968600	0.45181500	-1.39442900
C	3.32952300	-0.37691800	-0.71145200
C	3.08327100	-1.02821100	0.50355000
C	2.48879200	0.80997600	-1.12525100
C	3.86343500	-2.10920700	0.89164400
C	4.37100900	-0.81603900	-1.53242900
C	4.89056900	-2.52572600	0.05202600
C	5.16243500	-1.89716100	-1.15404700
C	0.67661600	-0.63080400	-2.16447000
H	2.46846000	1.56006900	-0.33387900
H	4.57587700	-0.31174700	-2.47052700
H	2.90296900	1.27272400	-2.02386800
H	5.97531600	-2.25484300	-1.77064900
H	3.69752900	-2.62767800	1.82576700
H	1.38090800	-1.30569300	-2.61871500
H	2.28251400	-0.68784900	1.15073300

C	-1.15780900	4.56141300	0.17390900
C	-0.72437000	4.20868700	-1.11852900
H	-2.18147900	4.63509200	0.50967200
H	-1.35022700	4.00765600	-1.97487400
N	-5.72887600	-3.68407300	0.46269600
N	5.72896400	-3.68409000	0.46291300
O	6.62194000	-4.02181500	-0.29690600
O	5.46124100	-4.21325900	1.52947600
O	-5.46112500	-4.21332800	1.52920800
O	-6.62180900	-4.02182800	-0.29715900

Complex 9 (anion, reduced):

Br	0.25026000	1.85824100	2.23801700
Ni	0.21991700	2.67571800	0.03558000
N	-1.11456900	0.22582400	-0.86265700
C	-3.47929100	-0.33680100	-0.27510600
C	-3.51632500	-1.11314800	0.89768400
C	-2.44748500	0.74028800	-0.45134000
C	-4.46198300	-2.10958600	1.06611300
C	-4.42987800	-0.59415800	-1.27659600
C	-5.40312700	-2.35086400	0.05032400
C	-5.38572500	-1.58590100	-1.12664900
C	0.03056700	0.93026600	-0.70445000
C	-0.85420700	-1.01473200	-1.42567600
C	0.46932100	3.83277500	-1.74058500

C	-0.84920100	4.18964100	-1.25823800
C	-0.69047200	4.78663900	-0.01274200
H	0.67754100	3.37652800	-2.69798500
H	-2.27542600	1.28432600	0.47847300
H	-4.41970900	0.00008900	-2.18576200
H	-2.77327600	1.45820700	-1.20820700
H	-6.12651900	-1.79033600	-1.88639200
H	-4.50577500	-2.71062100	1.96318700
H	-1.78038800	3.98397500	-1.76518500
H	-1.63198600	-1.73544200	-1.60393400
H	-2.79160800	-0.92303300	1.68287900
H	-1.47723500	5.10833800	0.65317600
N	1.01163600	0.12194800	-1.17159600
C	3.35813300	-0.62595800	-0.77166700
C	3.39838200	-1.04889600	0.56943900
C	2.44302800	0.49019400	-1.19713600
C	4.24634100	-2.06790900	0.96697400
C	4.19605800	-1.25844500	-1.70187600
C	5.07856200	-2.68701600	0.01964100
C	5.05349300	-2.27967800	-1.32152000
C	0.48492000	-1.08090800	-1.61969400
H	2.52623800	1.35262700	-0.53400300
H	4.17942800	-0.93831900	-2.73980000
H	2.69549700	0.81772800	-2.21017800
H	5.70833300	-2.77313700	-2.02535100

H	4.29327900	-2.40277400	1.99342300
H	1.10718100	-1.87489100	-1.99317400
H	2.75514800	-0.56726100	1.29924400
C	1.43400000	4.33407300	-0.82693700
C	0.72002800	4.82185000	0.28491500
H	2.50672400	4.25992900	-0.91994300
H	1.15180100	5.20156100	1.19906400
N	-6.38892300	-3.37575400	0.21734300
N	5.96656900	-3.73949700	0.42583700
O	6.69372000	-4.26638100	-0.44404800
O	5.97245600	-4.07783800	1.62788800
O	-6.38323100	-4.03675900	1.27942800
O	-7.21167400	-3.56203000	-0.70803100