LATTICE ENERGIES

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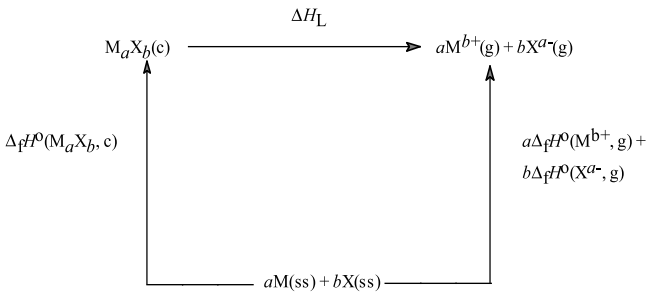
THERMOCHEMICAL CYCLE AND CALCULATED VALUES

Table 1 contains calculated values of the lattice energies (total lattice potential energies), U_{POT}, of crystalline salts, M_aX_b. U_{POT} is expressed in units of kilojoules per mole, kJ mol^{-1}. M and X can be either simple or complex ions. Substances are arranged by chemical class.

Also listed in the table is the lattice energy, U_{POT}^{BFHC}, obtained from the application of the Born - Fajans - Haber cycle (BHFC) described below, using the "Standard Thermochemical Properties of Chemical Substances" table in Section 5 of this *Handbook*, References 1 through 4, and certain other data which are given in Table 3 below.

The lattice enthalpy, ΔH_L, is given by the cycle:



where (ss) is the standard state of the element concerned.

The lattice enthalpy, ΔH_L, is obtained using the equation:

$$\Delta H_L = a\Delta_f H^\circ(M^{b+}, g) + b\Delta_f H^\circ(X^{a-}, g) - \Delta_f H^\circ(M_aX_b, c)$$

and is futher related to the total lattice potential energy, U_{POT}, by the relationship:

$$\Delta H_L = U_{POT} + \left[a\left(\frac{n_M}{2} - 2\right) + b\left(\frac{n_X}{2} - 2\right)\right]RT$$

where n_M and n_X equal 3 for monatomic ions, 5 for linear polyatomic ions and 6 for polyatomic non-linear ions.

METHOD OF ESTIMATION OF VALUES NOT TABULATED

In cases where the lattice energy is not tabulated and we want to furnish an estimate, then the Kapustinskii equation[5] can be used to obtain a value (in kJ mol^{-1}):

$$U_{POT} = \frac{121.4 z_a z_b \nu}{(r_a + r_b)}\left(1 - \frac{0.0345}{(r_a + r_b)}\right)$$

where z_a and z_b are the moduli of the charges on the ν ions in the lattice and r_a and r_b (in nm) are the thermochemical radii given in Table 2. The r_a for metal ions is taken to be the Goldschmidt[6] radius.

To cite an example, if we wish to estimate the lattice energy of the salt $[NH^+_4][HF^-_2]$ using the above procedure, we see that Table 2 gives the thermochemical radius (r_a) for NH^+_4 to be 0.136 nm and that for HF^-_2 (r_b) to be 0.172 nm. The lattice potential energy is then estimated to be 700 kJ mol^{-1} compared with the calculated value of 705 kJ mol^{-1} and the Born - Fajans - Haber cycle value of 658 kJ mol^{-1}.

References

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Table 1. Lattice Energies (kJ mol $^{-1}$)

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
Acetates		
$Li(CH_3COO)$	–	843
$Na(CH_3COO)$	828	807
$K(CH_3COO)$	749	726
$Rb(CH_3COO)$	715	–
$Cs(CH_3COO)$	682	–
Acetylides		
CaC_2	2911	2902
SrC_2	2788	2782
BaC_2	2647	2652
Azides		
LiN_3	861	875
NaN_3	770	784
KN_3	697	–
RbN_3	674	691
CsN_3	665	674
AgN_3	854	910
TlN_3	689	742
$Ca(N_3)_2$	2186	2316
$Sr(N_3)_2$	2056	2187
$Ba(N_3)_2$	2021	–
$Mn(N_3)_2$	2408	2348
$Cu(N_3)_2$	2730	2738
$Zn(N_3)_2$	2840	2970
$Cd(N_3)_2$	2446	2576
$Pb(N_3)_2$	–	2300
Bihalide Salts		
$LiHF_2$	821	847
$NaHF_2$	755	748
KHF_2	657	660
$RbHF_2$	627	631
$CsHF_2$	607	–
NH_4HF_2	705	658
$CsHCl_2$	601	–
Me_4NHCl_2	427	–
Et_4NHCl_2	346	–
Bu_4NHCl_2	290	–
Bicarbonates		
$NaHCO_3$	820	656
$KHCO_3$	741	573
$RbHCO_3$	707	522
$CsHCO_3$	678	520
NH_4HCO_3	–	577
Borides		
CaB_6	5146	–
SrB_6	5104	–
BaB_6	5021	–
YB_6	7447	–
LaB_6	7406	–
CeB_6	10083	–
PrB_6	7447	–
NdB_6	7447	–
PmB_6	7406	–
SmB_6	7447	–
EuB_6	5104	–
GdB_6	7489	–
TbB_6	7489	–
DyB_6	7489	–
HoB_6	7489	–
ErB_6	7489	–
TmB_6	7489	–
YbB_6	5146	–
LuB_6	7489	–
ThB_6	10167	–
Borohydrides		
$LiBH_4$	778	–
$NaBH_4$	703	694
KBH_4	655	638
$RbBH_4$	648	–
$CsBH_4$	628	–
Borohalides		
$LiBF_4$	699	749
$NaBF_4$	657	674
KBF_4	611	616
$RbBF_4$	577	590
$CsBF_4$	556	565
NH_4BF_4	582	–
$KBCl_4$	506	497
$RbBCl_4$	489	486
$CsBCl_4$	473	–
Carbonates		
Li_2CO_3	2523	2254
Na_2CO_3	2301	2016
K_2CO_3	2084	1846
Rb_2CO_3	2000	1783
Cs_2CO_3	1920	1722
$MgCO_3$	3138	3122
$CaCO_3$	2804	2811
$SrCO_3$	2720	2688
$BaCO_3$	2615	2554
$MnCO_3$	3046	3092
$FeCO_3$	3121	3169
$CoCO_3$	3443	3235
$CuCO_3$	3494	–
$ZnCO_3$	3121	3273
$CdCO_3$	2929	3052
$SnCO_3$	2904	–
$PbCO_3$	2728	2750
Cyanates		
LiNCO	849	–
NaNCO	807	816
KNCO	726	734
RbNCO	692	–
CsNCO	661	–
NH_4NCO	724	–
Cyanides		
LiCN	874	
NaCN	766	759
KCN	692	686
RbCN	638	–
CsCN	601	–
$Ca(CN)_2$	2268	2240
$Sr(CN)_2$	2138	–
$Ba(CN)_2$	2001	2009
NH_4CN	617	691
AgCN	(741)	935

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
$Zn(CN)_2$	2809	2817
$Cd(CN)_2$	2583	2591
Formates		
$Li(HCO_2)$	865	–
$Na(HCO_2)$	791	804
$K(HCO_2)$	713	722
$Rb(HCO_2)$	685	–
$Cs(HCO_2)$	651	–
$NH_4(HCO_2)$	715	–
Germanates		
Mg_2GeO_4	7991	–
Ca_2GeO_4	7301	7306
Sr_2GeO_4	6987	–
Ba_2GeO_4	6653	6643
Halates		
$LiBrO_3$	883	880
$NaBrO_3$	803	791
$KBrO_3$	740	722
$RbBrO_3$	720	705
$CsBrO_3$	694	681
$NaClO_3$	770	785
$KClO_3$	711	721
$RbClO_3$	690	703
$CsClO_3$	–	679
$LiIO_3$	975	974
$NaIO_3$	883	876
KIO_3	820	780
$RbIO_3$	791	–
$CsIO_3$	761	–
Halides		
LiF	1030	1049
LiCl	834	864
LiBr	788	820
LiI	730	764
NaF	910	930
NaCl	769	790
NaBr	732	754
NaI	682	705
KF	808	829
KCl	701	720
KBr	671	691
KI	632	650
RbF	774	795
RbCl	680	695
RbBr	651	668
RbI	617	632
CsF	744	759
CsCl	657	670
CsBr	632	647
CsI	600	613
FrF	715	–
FrCl	632	–
FrBr	611	–
FrI	582	–
CuCl	992	996
CuBr	969	978
CuI	948	966
AgF	953	974
AgCl	910	918
AgBr	897	905

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
AgI	881	892
AuCl	1013	1066
AuBr	1029	1059
AuI	1027	1070
InCl	–	764
InBr	–	767
InI	–	733
TlF	–	850
TlCl	738	751
TlBr	720	734
TlI	692	710
Me_4NCl	566	–
Me_4NBr	553	–
Me_4NI	544	–
PH_4Br	616	–
PH_4I	590	–
BeF_2	3464	3526
$BeCl_2$	3004	3033
$BeBr_2$	2950	2914
BeI_2	2780	2813
MgF_2	2926	2978
$MgCl_2$	2477	2540
$MgBr_2$	2406	2451
MgI_2	2293	2340
CaF_2	2640	2651
$CaCl_2$	2268	2271
$CaBr_2$	2132	–
CaI_2	1971	2087
SrF_2	2476	2513
$SrCl_2$	2142	2170
SrI_2	1984	1976
BaF_2	2347	2373
$BaCl_2$	2046	2069
$BaBr_2$	1971	1995
BaI_2	1862	1890
RaF_2	2284	–
$RaCl_2$	2004	–
$RaBr_2$	1929	–
RaI_2	1803	–
$ScCl_2$	2380	–
$ScBr_2$	2291	–
ScI_2	2201	–
TiF_2	2724	–
$TiCl_2$	2439	2514
$TiBr_2$	2360	2430
TiI_2	2259	2342
VCl_2	2607	2593
VBr_2	–	2534
VI_2	–	2470
CrF_2	2778	2939
$CrCl_2$	2540	2601
$CrBr_2$	2377	2536
CrI_2	2269	2440
$MoCl_2$	2737	2746
$MoBr_2$	2742	2753
MoI_2	2630	–
MnF_2	2644	–
$MnCl_2$	2510	2551
$MnBr_2$	2448	2482
MnI_2	2212	–
FeF_2	2849	2967

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
$FeCl_2$	2569	2641
$FeBr_2$	2515	2577
FeI_2	2439	2491
CoF_2	3004	3042
$CoCl_2$	2707	2706
$CoBr_2$	2640	2643
CoI_2	2569	2561
NiF_2	3098	3089
$NiCl_2$	2753	2786
$NiBr_2$	2729	2721
NiI_2	2607	2637
$PdCl_2$	2778	2818
$PdBr_2$	2741	2751
PdI_2	2748	2760
CuF_2	3046	3102
$CuCl_2$	2774	2824
$CuBr_2$	2715	2774
CuI_2	2640	–
AgF_2	2942	2967
ZnF_2	3021	3053
$ZnCl_2$	2703	2748
$ZnBr_2$	2648	2689
ZnI_2	2581	2619
CdF_2	2809	2830
$CdCl_2$	2552	2565
$CdBr_2$	2507	2517
CdI_2	2441	2455
HgF_2	2757	–
$HgCl_2$	2657	2664
$HgBr_2$	2628	2639
HgI_2	2628	2624
SnF_2	2551	–
$SnCl_2$	2297	2310
$SnBr_2$	2251	2256
SnI_2	2193	2206
PbF_2	2535	2543
$PbCl_2$	2270	2282
$PbBr_2$	2219	2230
PbI_2	2163	2177
ScF_3	5492	5540
$ScCl_3$	4874	4901
$ScBr_3$	4729	4761
ScI_3	4640	–
YF_3	4983	–
YCl_3	4506	4524
YI_3	4240	4258
TiF_3	5644	–
$TiCl_3$	5134	5153
$TiBr_3$	5012	5023
TiI_3	4845	–
$ZrCl_3$	–	4791
$ZrBr_3$	–	4758
ZrI_3	–	4591
VF_3	5895	–
VCl_3	5322	5329
VBr_3	5214	5224
VI_3	5121	5136
$NbCl_3$	5062	–
$NbBr_3$	4980	–
NbI_3	4860	–
CrF_3	6033	6065

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
$CrCl_3$	5518	5529
$CrBr_3$	5355	–
CrI_3	5275	5294
MoF_3	6459	–
$MoCl_3$	5246	5253
$MoBr_3$	5156	–
MoI_3	5073	–
MnF_3	6017	–
$MnCl_3$	5544	–
$MnBr_3$	5448	–
MnI_3	5330	–
$TcCl_3$	5270	–
$TcBr_3$	5215	–
TcI_3	5188	–
FeF_3	5870	–
$FeCl_3$	5364	5436
$FeBr_3$	5333	5347
FeI_3	5117	–
$RuCl_3$	5245	5257
$RuBr_3$	5223	5232
RuI_3	5222	5235
CoF_3	5991	–
$RhCl_3$	5641	5665
IrF_3	(6112)	–
$IrBr_3$	(4794)	–
NiF_3	(6111)	–
AuF_3	(5777)	–
$AuCl_3$	(4605)	–
$ZnCl_3$	5832	–
$ZnBr_3$	5732	–
ZnI_3	5636	–
AlF_3	5924	6252
$AlCl_3$	5376	5513
$AlBr_3$	5247	5360
AlI_3	5070	5227
GaF_3	5829	6238
$GaCl_3$	5217	5665
$GaBr_3$	4966	5569
GaI_3	4611	5496
$InCl_3$	4736	5183
$InBr_3$	4535	5117
InI_3	4234	5001
TlF_3	5493	–
$TlCl_3$	5258	5278
$TlBr_3$	5171	–
TlI_3	5088	–
$AsBr_3$	5497	5365
AsI_3	4824	5295
SbF_3	5295	5324
$SbCl_3$	5032	4857
$SbBr_3$	4954	4776
SbI_3	4867	4692
$BiCl_3$	4689	4707
BiI_3	3774	–
LaF_3	4682	–
$LaCl_3$	4263	4242
$LaBr_3$	4209	–
LaI_3	3916	3986
$CeCl_3$	4394	4348
CeI_3	–	4061
$PrCl_3$	4322	4387

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
PrI_3	–	4101
$NdCl_3$	4343	4415
$SmCl_3$	4376	4450
$EuCl_3$	4393	4490
$GdCl_3$	4406	4495
$DyCl_3$	4481	4529
$HoCl_3$	4501	4572
$ErCl_3$	4527	4591
$TmCl_3$	4548	4608
TmI_3	–	4340
$YbCl_3$	–	4651
$AcCl_3$	4096	–
UCl_3	4243	–
$NpCl_3$	4268	–
$PuCl_3$	4289	–
$PuBr_3$	(3959)	–
$AmCl_3$	4293	–
TiF_4	10012	9908
$TiCl_4$	9431	–
$TiBr_4$	9288	9059
TiI_4	9108	8918
ZrF_4	8853	8971
$ZrCl_4$	8021	8144
$ZrBr_4$	7661	7984
ZrI_4	7155	7801
MoF_4	8795	–
$MoCl_4$	8556	9603
$MoBr_4$	8510	9500
MoI_4	8427	–
$SnCl_4$	8355	8930
$SnBr_4$	7970	8852
PbF_4	9519	–
CrF_2Cl	5795	–
CrF_2Br	5753	–
CrF_2I	5669	–
$CrCl_2Br$	5448	–
$CrCl_2I$	5381	5429
$CrBr_2I$	5330	5370
CuFCl	2891	–
CuFBr	2853	–
CuFI	2803	–
CuClBr	2753	–
CuClI	2694	–
CuBrI	2669	–
FeF_2Cl	5711	–
FeF_2Br	5653	–
FeF_2I	5569	–
$FeCl_2Br$	5339	–
$FeCl_2I$	5272	–
$FeBr_2I$	5209	–
$LiIO_2F_2$	845	–
$NaIO_2F_2$	766	756
KIO_2F_2	699	689
$RbIO_2F_2$	674	–
$CsIO_2F_2$	636	–
$NH_4IO_2F_2$	678	–
$AgIO_2F_2$	736	685
Hydrides		
LiH	916	918
NaH	807	807
KH	711	713
RbH	686	684
CsH	648	653
VH	1184	(1344)
NbH	1163	(1633)
PdH	979	1368
CuH	828	1254
TiH	996	1407
ZrH	916	1590
HfH	904	–
LaH	828	–
TaH	1021	–
CrH	1050	–
NiH	929	–
PtH	937	–
AgH	941	–
AuH	1033	1108
TlH	745	–
GeH	950	–
PbH	778	–
BeH_2	3205	3306
MgH_2	2791	2718
CaH_2	2410	2406
SrH_2	2250	2265
BaH_2	2121	2133
ScH_2	2711	2744
YH_2	(2598)	2733
LaH_2	2380	2522
CeH_2	2414	2509
PrH_2	2448	2405
NdH_2	2464	2394
PmH_2	2519	–
SmH_2	2510	2389
GdH_2	2494	2651
AcH_2	2372	–
ThH_2	2711	2738
PuH_2	2519	–
AmH_2	2544	–
TiH_2	2866	2864
ZrH_2	2711	2999
CuH_2	2941	–
ZnH_2	2870	–
HgH_2	2707	–
AlH_3	5924	5969
FeH_3	5724	–
ScH_3	5439	–
YH_3	5063	4910
LaH_3	4895	4493
FeH_3	5724	–
GaH_3	5690	–
InH_3	5092	–
TlH_3	5092	–
Hydroselenides		
NaHSe	703	732
KHSe	644	712
RbHSe	623	689
CsHse	598	669
Hydrosulphides		
LiHS	768	862
NaHS	723	771
RbHS	655	682

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
CsHS	628	657
NH_4HS	661	718
$Ca(HS)_2$	2184	(2171)
$Sr(HS)_2$	2063	–
$Ba(HS)_2$	1979	(1956)
Hydroxides		
LiOH	1021	1028
NaOH	887	892
KOH	789	796
RbOH	766	765
CsOH	721	732
$Be(OH)_2$	3477	3620
$Mg(OH)_2$	2870	2998
$Ca(OH)_2$	2506	2637
$Sr(OH)_2$	2330	2474
$Ba(OH)_2$	2142	2330
$Ti(OH)_2$	–	2953
$Mn(OH)_2$	2909	3008
$Fe(OH)_2$	2653	3044
$Co(OH)_2$	2786	3109
$Ni(OH)_2$	2832	3186
$Pd(OH)_2$	–	3189
$Cu(OH)_2$	2870	3229
CuOH	1006	–
AgOH	918	845
AuOH	1033	–
TlOH	705	874
$Zn(OH)_2$	2795	3151
$Cd(OH)_2$	2607	2909
$Hg(OH)_2$	2669	–
$Sn(OH)_2$	2489	2721
$Pb(OH)_2$	2376	–
$Sc(OH)_3$	5063	5602
$Y(OH)_3$	4707	–
$La(OH)_3$	4443	–
$Cr(OH)_3$	5556	6299
$Mn(OH)_3$	6213	–
$Al(OH)_3$	5627	–
$Ga(OH)_3$	5732	6368
$In(OH)_3$	5280	–
$Tl(OH)_3$	5314	–
$Ti(OH)_4$	9456	–
$Zr(OH)_4$	8619	–
$Mn(OH)_4$	10933	–
$Sn(OH)_4$	9188	9879
Imides		
CaNH	3293	–
SrNH	3146	–
BaNH	2975	–
Metavanadates		
Li_3VO_4	3945	–
Na_3VO_4	3766	–
K_3VO_4	3376	–
Rb_3VO_4	3243	–
Cs_3VO_4	3137	–
Nitrates		
$LiNO_3$	848	854
$NaNO_3$	755	763
KNO_3	685	694
$RbNO_3$	662	671

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
$CsNO_3$	648	650
$AgNO_3$	820	832
$TlNO_3$	690	707
$Mg(NO_3)_2$	2481	2521
$Ca(NO_3)_2$	2268	2247
$Sr(NO_3)_2$	2176	2151
$Ba(NO_3)_2$	2062	2035
$Mn(NO_3)_2$	2318	2478
$Fe(NO_3)_2$	–	(2580)
$Co(NO_3)_2$	2560	2647
$Ni(NO_3)_2$	–	2729
$Cu(NO_3)_2$	–	2739
$Zn(NO_3)_2$	2376	2649
$Cd(NO_3)_2$	2238	2462
$Sn(NO_3)_2$	2155	2254
$Pb(NO_3)_2$	2067	2208
Nitrides		
ScN	7547	7506
LaN	6876	6793
TiN	8130	8033
ZrN	7633	7723
VN	8283	8233
NbN	7939	8022
CrN	8269	8358
Nitrites		
$NaNO_2$	774	772
KNO_2	699	687
$RbNO_2$	724	765
$CsNO_2$	690	–
Oxides		
Li_2O	2799	2814
Na_2O	2481	2478
K_2O	2238	2232
Rb_2O	2163	2161
Cs_2O	2131	2063
Cu_2O	3273	3189
Ag_2O	3002	2910
Tl_2O	2659	2575
LiO_2	(878)	(872)
NaO_2	799	821
KO_2	741	751
RbO_2	706	721
CsO_2	679	696
Li_2O_2	2592	2557
Na_2O_2	2309	22717
K_2O_2	2114	2064
Rb_2O_2	2025	1994
Cs_2O_2	1948	1512
MgO_2	3356	3526
CaO_2	3144	3132
SrO_2	3037	2977
KO_3	697	707
BeO	4514	4443
MgO	3795	3791
CaO	3414	3401
SrO	3217	3223
BaO	3029	3054
TiO	3832	3811
VO	3932	3863
MnO	3724	3745

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
FeO	3795	3865
CoO	3837	3910
NiO	3908	4010
PdO	3736	–
CuO	4135	4050
ZnO	4142	3971
CdO	3806	–
HgO	3907	–
GeO	3919	–
SnO	3652	–
PbO	3520	–
Sc_2O_3	13557	13708
Y_2O_3	12705	–
La_2O_3	12452	–
Ce_2O_3	12661	–
Pr_2O_3	12703	–
Nd_2O_3	12736	–
Pm_2O_3	12811	–
Sm_2O_3	12878	–
Eu_2O_3	12945	–
Gd_2O_3	12996	–
Tb_2O_3	13071	–
Dy_2O_3	13138	–
Ho_2O_3	13180	–
Er_2O_3	13263	–
Tm_2O_3	13322	–
Yb_2O_3	13380	–
Lu_2O_3	13665	–
Ac_2O_3	12573	–
Ti_2O_3	–	14149
V_2O_3	15096	14520
Cr_2O_3	15276	14957
Mn_2O_3	15146	15035
Fe_2O_3	14309	14774
Al_2O_3	15916	–
Ga_2O_3	15590	15220
In_2O_3	13928	–
Pb_2O_3	(14841)	–
CeO_2	9627	–
ThO_2	10397	–
PaO_2	10573	–
VO_2(g)	10644	–
NpO_2	10707	–
PuO_2	10786	–
AmO_2	10799	–
CmO_2	10832	–
TiO_2	12150	–
ZrO_2	11188	–
MoO_2	11648	–
MnO_2	12970	–
SiO_2	13125	–
GeO_2	12828	–
SnO_2	11807	–
PbO_2	11217	–
Perchlorates		
$LiClO_4$	709	715
$NaClO_4$	643	641
$KClO_4$	599	595
$RbClO_4$	564	576
$CsClO_4$	636	550
NH_4ClO_4	583	580
$Ca(ClO_4)_2$	1958	1971
$Sr(ClO_4)_2$	1862	1862
$Ba(ClO_4)_2$	1795	1769
Permanganates		
$NaMnO_4$	661	–
$KMnO_4$	607	–
$RbMnO_4$	586	–
$CsMnO_4$	565	–
$Ca(MnO_4)_2$	1937	–
$Sr(MnO_4)_2$	1845	–
$Ba(MnO_4)_2$	1778	–
Phosphates		
$Mg_3(PO_4)_2$	11632	11407
$Ca_3(PO_4)_2$	10602	10479
$Sr_3(PO_4)_2$	10125	10075
$Ba_3(PO_4)_2$	9652	9654
$MnPO_4$	7397	–
$FePO_4$	7251	7300
BPO_4	8201	–
$AlPO_4$	7427	7507
$GaPO_4$	7381	–
Selenides		
Li_2Se	2364	–
Na_2Se	2130	–
K_2Se	1933	–
Rb_2Se	1837	–
Cs_2Se	1745	–
Ag_2Se	2686	–
Tl_2Se	2209	–
BeSe	3431	–
MgSe	3071	–
CaSe	2858	2862
SrSe	2736	–
BaSe	2611	–
MnSe	3176	–
Selenites		
Li_2SeO_3	2171	–
Na_2SeO_3	1950	1916
K_2SeO_3	1774	1749
Rb_2SeO_3	1715	1675
Cs_2SeO_3	1640	–
Tl_2SeO_3	1879	–
Ag_2SeO_3	2113	2148
$BeSeO_3$	3322	–
$MgSeO_3$	3012	2998
$CaSeO_3$	2732	–
$SrSeO_3$	2586	2588
$BaSeO_3$	2460	2451
Selenates		
Li_2SeO_4	2054	–
Na_2SeO_4	1879	–
K_2SeO_4	1732	–
Rb_2SeO_4	1686	–
Cs_2SeO_4	1615	–
Cu_2SeO_4	2201	–
Ag_2SeO_4	2033	–
Tl_2SeO_4	1766	–
Hg_2SeO_4	2163	–
$BeSeO_4$	3448	–

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
$MgSeO_4$	2895	–
$CaSeO_4$	2632	–
$SrSeO_4$	2489	–
Sulphides		
Li_2S	2464	2472
Na_2S	2192	2203
K_2S	1979	(2052)
Rb_2S	1929	1949
Cs_2S	1892	1850
$(NH_4)_2S$	2008	(2026)
Cu_2S	2786	2865
Ag_2S	2606	2677
Au_2S	2908	–
Tl_2S	2298	2258
Sulphates		
Li_2SO_4	2229	2142
Na_2SO_4	1827	1938
K_2SO_4	1700	1796
Rb_2SO_4	1636	1748
Cs_2SO_4	1596	1658
$(NH_4)_2SO_4$	1766	1777
Cu_2SO_4	2276	2166
Ag_2SO_4	2104	1989
Tl_2SO_4	1828	1722
Hg_2SO_4	–	2127
$CaSO_4$	2489	2480
$SrSO_4$	2577	2484
$BaSO_4$	2469	2374
$MnSO_4$	2920	2825
Ternary Salts		
Cs_2CuCl_4	1393	–
Rb_2ZnCl_4	1529	–
Cs_2ZnCl_4	1492	–
Rb_2ZnBr_4	1498	–
Cs_2ZnBr_4	1454	–
Cs_2ZnI_4	1386	–
$CsGaCl_4$	494	–
$NaAlCl_4$	556	–
$CsAlCl_4$	486	–
$NaFeCl_4$	492	–
Rb_2CoCl_4	1447	–
Cs_2CoCl_4	1391	–
K_2PtCl_4	1574	1550
Cs_2GeF_6	1573	–
$(NH_4)_2GeF_6$	1657	–
Cs_2GeCl_6	1404	1419
K_2HfCl_6	1345	1461
K_2IrCl_6	1442	1440
Na_2MoCl_6	1526	1504
K_2MoCl_6	1418	1412
Rb_2MoCl_6	1399	1399
Cs_2MoCl_6	1347	1347
K_2NbCl_6	1375	1398
Rb_2NbCl_6	1371	1385
Cs_2NbCl_6	1381	1344
K_2OsCl_6	1447	1447
Cs_2OsCl_6	1409	–
K_2OsBr_6	1396	–
K_2PdCl_6	1481	1493
Rb_2PdCl_6	1449	–
Cs_2PdCl_6	1426	–
Rb_2PbCl_6	1343	1343
Cs_2PbCl_6	1344	–
$(NH_4)_2PbCl_6$	1355	–
K_2PtCl_6	1468	1471
Rb_2PtCl_6	1464	–
Cs_2PtCl_6	1444	–
$(NH_4)_2PtCl_6$	1468	–
Tl_2PtCl_6	1546	–
Ag_2PtCl_6	1773	1881
$BaPtCl_6$	2047	2070
K_2PtBr_6	1423	1392
Ag_2PtBr_6	1791	2276
K_2PtI_6	1421	–
K_2ReCl_6	1416	1442
Rb_2ReCl_6	1414	–
Cs_2ReCl_6	1398	–
K_2ReBr_6	1375	1375
K_2SiF_6	1670	1765
Rb_2SiF_6	1639	1673
Cs_2SiF_6	1604	1498
Tl_2SiF_6	1675	–
K_2SnCl_6	1363	1390
Rb_2SnCl_6	1361	1363
Cs_2SnCl_6	1358	–
Tl_2SnCl_6	1437	–
$(NH_4)_2SnCl_6$	1370	1344
Rb_2SnBr_6	1309	–
Cs_2SnBr_6	1306	–
Rb_2SnI_6	1226	–
Cs_2SnBr_6	1243	–
K_2TeCl_6	1318	1320
Rb_2TeCl_6	1321	–
Cs_2TeCl_6	1323	–
Tl_2TeCl_6	1392	–
$(NH_4)_2TeCl_6$	1318	–
K_2RuCl_6	1451	–
Rb_2CoF_6	1688	–
Cs_2CoF_6	1632	–
K_2NiF_6	1721	–
Rb_2NiF_6	1688	–
Rb_2SbCl_6	1357	–
Rb_2SeCl_6	1409	–
Cs_2SeCl_6	1397	–
$(NH_4)_2SeCl_6$	1420	–
$(NH_4)_2PoCl_6$	1338	–
Cs_2PoBr_6	1286	–
Cs_2CrF_6	1603	–
Rb_2MnF_6	1688	–
Cs_2MnF_6	1620	–
K_2MnCl_6	1462	–
Rb_2MnCl_6	1451	–
$(NH_4)_2MnCl_6$	1464	–
Cs_2TeBr_6	1306	–
Cs_2TeI_6	1246	–
K_2TiCl_6	1412	1447
Rb_2TiCl_6	1415	1416
Cs_2TiCl_6	1402	1384
Tl_2TiCl_6	1560	1553
K_2TiBr_6	1379	1379
Rb_2TiBr_6	1341	1331

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
Cs_2TiBr_6	1339	1306
Na_2UBr_6	1504	–
K_2UBr_6	1484	–
Rb_2UBr_6	1473	–
Cs_2UBr_6	1459	–
K_2WCl_6	1398	1423
Rb_2WCl_6	1397	1434
Cs_2WCl_6	1392	1366
K_2WBr_6	1408	1408
Rb_2WBr_6	1361	1391
Cs_2WBr_6	1362	1332
K_2ZrCl_6	1339	1371
Rb_2ZrCl_6	1341	–
Cs_2ZrCl_6	1339	1307
Tellurides		
Li_2Te	2212	–
Na_2Te	1997	2095
K_2Te	1830	–
Rb_2Te	1837	–
Cs_2Te	1745	–
Cu_2Te	2706	2683
Ag_2Te	2607	2600
Tl_2Te	2084	2172
BeTe	3319	–
MgTe	2878	3081
CaTe	2721	–

Substance	Calc. U_{POT}	U_{POT}^{BHFC}
Thiocyanates		
LiCNS	764	(765)
NaCNS	682	682
KCNS	623	616
RbCNS	623	619
CsCNS	623	568
NH4CNS	605	611
Ca(CNS)2	2184	2118
Sr(CNS)2	2063	1957
Ba(CNS)2	1979	1852
Mn(CNS)2	2280	2351
Zn(CNS)2	2335	2560
Cd(CNS)2	2201	2374
Hg(CNS)2	2146	2492
Sn(CNS)2	2117	2142
Pb(CNS)2	2058	–
Vanadates		
LiVO3	810	–
NaVO3	761	–
KVO3	686	–
RbVO3	657	–
CsVO3	628	–

TABLE 2. Thermochemical Radii (nm)

Ion	Radius	
Singly Charged Anions		
AgF_4^-	0.231	± 0.019
$AlBr_4^-$	0.321	± 0.023
$AlCl_4^-$	0.317	± 0.019
AlF_4^-	0.214	± 0.023
AlH_4^-	0.226	± 0.019
AlI_4^-	0.374	± 0.019
AsF_6^-	0.243	± 0.019
AsO_2^-	0.211	± 0.019
$Au(CN)_2^-$	0.266	± 0.019
$AuCl_4^-$	0.288	± 0.019
AuF_4^-	0.240	± 0.019
AuF_6^-	0.235	± 0.038
$B(OH)_4^-$	0.229	± 0.019
BF_4^-	0.205	± 0.019
BH_4^-	0.205	± 0.019
Br^-	0.190	± 0.019
BrF_4^-	0.231	± 0.019
BrO_3^-	0.214	± 0.019
$CF_3SO_3^-$	0.230	± 0.049
$CH_3CO_2^-$	0.194	± 0.019
Cl^-	0.168	± 0.019
ClO_2^-	0.195	± 0.019
ClO_3^-	0.208	± 0.019
ClO_4^-	0.225	± 0.019
$ClS_2O_6^-$	0.260	± 0.049
CN^-	0.187	± 0.023
$Cr_3O_8^-$	0.276	± 0.019
$CuBr_4^-$	0.315	± 0.019
F^-	0.126	± 0.019
$FeCl_4^-$	0.317	± 0.019

Ion	Radius	
$GaCl_4^-$	0.328	± 0.019
H^-	0.148	± 0.019
$H_2AsO_4^-$	0.227	± 0.019
$H_2PO_4^-$	0.213	± 0.019
HCO_2^-	0.200	± 0.019
HCO_3^-	0.207	± 0.019
HF_2^-	0.172	± 0.019
HSO_4^-	0.221	± 0.019
I^-	0.211	± 0.019
I_2Br^-	0.261	± 0.019
I_3^-	0.272	± 0.019
I_4^-	0.300	± 0.019
IBr_2^-	0.251	± 0.019
ICl_2^-	0.235	± 0.019
ICl_4^-	0.307	± 0.019
$IO_2F_2^-$	0.233	± 0.019
IO_3^-	0.218	± 0.019
IO_4^-	0.231	± 0.019
IrF_6^-	0.242	± 0.019
MnO_4^-	0.220	± 0.019
MoF_6^-	0.241	± 0.019
$MoOF_5^-$	0.241	± 0.019
N_3^-	0.180	± 0.019
NCO^-	0.193	± 0.019
$NbCl_6^-$	0.338	± 0.049
NbF_6^-	0.254	± 0.019
$Nb_2F_{11}^-$	0.311	± 0.038
NbO_3^-	0.194	± 0.019
NH_2^-	0.168	± 0.019
$NH_2CH_2COO^-$	0.252	± 0.019
NO_2^-	0.187	± 0.019

Ion	Radius	
NO_3^-	0.200	± 0.019
O_2^-	0.165	± 0.019
O_3^-	0.199	± 0.034
OH^-	0.152	± 0.019
OsF_6^-	0.252	± 0.020
PaF_6^-	0.249	± 0.019
PdF_6^-	0.252	± 0.019
PF_6^-	0.242	± 0.019
PO_3^-	0.204	± 0.019
PtF_6^-	0.247	± 0.019
PuF_5^-	0.239	± 0.019
ReF_6^-	0.240	± 0.019
ReO_4^-	0.227	± 0.019
RuF_6^-	0.242	± 0.019
S_6^-	0.305	± 0.019
SCN^-	0.209	± 0.019
$SbCl_6^-$	0.320	± 0.019
SbF_6^-	0.252	± 0.019
$Sb_2F_{11}^-$	0.312	± 0.038
$Sb_3F_{14}^-$	0.374	± 0.038
$SeCl_5^-$	0.258	± 0.038
$SeCN^-$	0.230	± 0.019
SeH^-	0.195	± 0.019
SH^-	0.191	± 0.019
SO_3F^-	0.214	± 0.019
$S_3N_3^-$	0.231	± 0.038
$S_3N_3O_4^-$	0.252	± 0.038
$TaCl_6^-$	0.352	± 0.019
TaF_6^-	0.250	± 0.019
TaO_3^-	0.192	± 0.019
UF_6^-	0.301	± 0.019
VF_6^-	0.235	± 0.019
VO_3^-	0.201	± 0.019
WCl_6^-	0.337	± 0.019
WF_6^-	0.246	± 0.019
WOF_5^-	0.241	± 0.019
Doubly Charged Anions		
AmF_6^{2-}	0.255	± 0.019
$Bi_2Br_8^{2-}$	0.392	± 0.055
$Bi_6Cl_{20}^{2-}$	0.501	± 0.073
$CdCl_4^{2-}$	0.307	± 0.019
$CeCl_6^{2-}$	0.352	± 0.019
CeF_6^{2-}	0.249	± 0.019
CO_3^{2-}	0.189	± 0.019
$CoCl_4^{2-}$	0.306	± 0.019
CoF_4^{2-}	0.209	± 0.019
CoF_6^{2-}	0.256	± 0.019
$Cr_2O_7^{2-}$	0.292	± 0.019
CrF_6^{2-}	0.253	± 0.019
CrO_4^{2-}	0.229	± 0.019
$CuCl_4^{2-}$	0.304	± 0.019
CuF_4^{2-}	0.213	± 0.019
$GeCl_6^{2-}$	0.335	± 0.019
GeF_6^{2-}	0.244	± 0.019
HfF_6^{2-}	0.248	± 0.019
HgI_4^{2-}	0.377	± 0.019
$IrCl_6^{2-}$	0.332	± 0.019
$MnCl_6^{2-}$	0.314	± 0.031
MnF_4^{2-}	0.219	± 0.019
MnF_6^{2-}	0.241	± 0.019
$MoBr_6^{2-}$	0.364	± 0.019

Ion	Radius	
$MoCl_6^{2-}$	0.338	± 0.019
MoF_6^{2-}	0.274	± 0.019
MoO_4^{2-}	0.231	± 0.019
$NbCl_6^{2-}$	0.343	± 0.019
NH^{2-}	0.128	± 0.019
$Ni(CN)_4^{2-}$	0.322	± 0.019
NiF_4^{2-}	0.211	± 0.019
NiF_6^{2-}	0.249	± 0.019
O^{2-}	0.141	± 0.019
O_2^{2-}	0.167	± 0.019
$OsBr_6^{2-}$	0.365	± 0.019
$OsCl_6^{2-}$	0.336	± 0.019
OsF_6^{2-}	0.276	± 0.019
$PbCl_4^{2-}$	0.279	± 0.019
$PbCl_6^{2-}$	0.347	± 0.019
PbF_6^{2-}	0.268	± 0.019
$PdBr_6^{2-}$	0.354	± 0.019
$PdCl_4^{2-}$	0.313	± 0.019
$PdCl_6^{2-}$	0.333	± 0.019
PdF_6^{2-}	0.252	± 0.019
$PoBr_6^{2-}$	0.380	± 0.019
PoI_6^{2-}	0.428	± 0.019
$Pt(NO_2)_3Cl_3^{2-}$	0.364	± 0.019
$Pt(NO_2)_4Cl_2^{2-}$	0.383	± 0.019
$Pt(OH)_2^{2-}$	0.333	± 0.019
$Pt(SCN)_6^{2-}$	0.451	± 0.019
$PtBr_4^{2-}$	0.324	± 0.019
$PtBr_6^{2-}$	0.363	± 0.019
$PtCl_4^{2-}$	0.307	± 0.019
$PtCl_6^{2-}$	0.333	± 0.019
PtF_6^{2-}	0.245	± 0.019
$PuCl_6^{2-}$	0.349	± 0.019
$ReBr_6^{2-}$	0.371	± 0.019
$ReCl_6^{2-}$	0.337	± 0.019
ReF_6^{2-}	0.256	± 0.019
ReF_8^{2-}	0.276	± 0.019
ReH_9^{2-}	0.257	± 0.019
ReI_6^{2-}	0.421	± 0.026
RhF_6^{2-}	0.240	± 0.019
$RuCl_6^{2-}$	0.336	± 0.019
RuF_6^{2-}	0.248	± 0.019
S^{2-}	0.189	± 0.019
$S_2O_3^{2-}$	0.251	± 0.019
$S_2O_4^{2-}$	0.262	± 0.019
$S_2O_5^{2-}$	0.270	± 0.019
$S_2O_6^{2-}$	0.283	± 0.019
$S_2O_7^{2-}$	0.275	± 0.019
$S_2O_8^{2-}$	0.291	± 0.019
$S_3O_6^{2-}$	0.302	± 0.019
$S_4O_6^{2-}$	0.325	± 0.019
$S_6O_6^{2-}$	0.382	± 0.019
ScF_6^{2-}	0.276	± 0.019
Se^{2-}	0.181	± 0.019
$SeBr_6^{2-}$	0.363	± 0.019
$SeCl_6^{2-}$	0.336	± 0.019
SeO_4^{2-}	0.229	± 0.019
SiF_6^{2-}	0.248	± 0.019
SiO_3^{2-}	0.195	± 0.019
SmF_4^{2-}	0.218	± 0.019
$Sn(OH)_6^{2-}$	0.279	± 0.020
$SnBr_6^{2-}$	0.374	± 0.019

Ion	Radius	
$SnCl_6^{2-}$	0.345	± 0.019
SnF_6^{2-}	0.265	± 0.019
SnI_6^{2-}	0.427	± 0.019
SO_3^{2-}	0.204	± 0.019
SO_4^{2-}	0.218	± 0.019
$TcBr_6^{2-}$	0.363	± 0.019
$TcCl_6^{2-}$	0.337	± 0.019
TcF_6^{2-}	0.244	± 0.019
TcH_9^{2-}	0.260	± 0.019
TcI_6^{2-}	0.419	± 0.019
Te^{2-}	0.220	± 0.019
$TeBr_6^{2-}$	0.383	± 0.019
$TeCl_6^{2-}$	0.353	± 0.019
TeI_6^{2-}	0.430	± 0.019
TeO_4^{2-}	0.238	± 0.019
$Th(NO_3)_6^{2-}$	0.424	± 0.019
$ThCl_6^{2-}$	0.360	± 0.019
ThF_6^{2-}	0.263	± 0.019
$TiBr_6^{2-}$	0.356	± 0.019
$TiCl_6^{2-}$	0.335	± 0.019
TiF_6^{2-}	0.252	± 0.019
UCl_6^{2-}	0.354	± 0.019
UF_6^{2-}	0.256	± 0.019
VO_3^{2-}	0.204	± 0.019
WBr_6^{2-}	0.363	± 0.019
WCl_6^{2-}	0.339	± 0.019
WO_4^{2-}	0.237	± 0.019
$WOCl_5^{2-}$	0.334	± 0.019
$ZnBr_4^{2-}$	0.335	± 0.019
$ZnCl_4^{2-}$	0.306	± 0.019
ZnF_4^{2-}	0.219	± 0.019
ZnI_4^{2-}	0.384	± 0.019
$ZrBr_4^{2-}$	0.334	± 0.019
$ZrCl_4^{2-}$	0.306	± 0.019
$ZrCl_6^{2-}$	0.348	± 0.019
ZrF_6^{2-}	0.258	± 0.019
Multi-Charged Anions		
AlH_6^{3-}	0.256	± 0.042
AsO_4^{3-}	0.237	± 0.042
$CdBr_6^{4-}$	0.374	± 0.038
$CdCl_6^{4-}$	0.352	± 0.038
CeF_6^{3-}	0.278	± 0.038
CeF_7^{3-}	0.282	± 0.038
$Co(CN)_6^{3-}$	0.349	± 0.038
$Co(NO_2)_6^{3-}$	0.343	± 0.038
$CoCl_5^{3-}$	0.320	± 0.038
CoF_6^{3-}	0.258	± 0.042
$Cr(CN)_6^{3-}$	0.351	± 0.038
CrF_6^{3-}	0.254	± 0.042
$Cu(CN)_4^{3-}$	0.312	± 0.038
$Fe(CN)_6^{3-}$	0.347	± 0.038
FeF_6^{3-}	0.298	± 0.042
HfF_7^{3-}	0.277	± 0.042
InF_6^{3-}	0.268	± 0.038
$Ir(CN)_6^{3-}$	0.347	± 0.038
$Ir(NO_2)_6^{3-}$	0.338	± 0.038
$Mn(CN)_6^{3-}$	0.350	± 0.038
$Mn(CN)_6^{5-}$	0.401	± 0.042
$MnCl_6^{4-}$	0.349	± 0.038
N^{3-}	0.180	± 0.042
$Ni(NO_2)_6^{3-}$	0.342	± 0.038
$Ni(NO_2)_6^{4-}$	0.383	± 0.038
NiF_6^{3-}	0.250	± 0.042
O^{3-}	0.288	± 0.038
P^{3-}	0.224	± 0.042
PaF_8^{3-}	0.299	± 0.042
PO_4^{3-}	0.230	± 0.042
PrF_6^{3-}	0.281	± 0.038
$Rh(NO_2)_6^{3-}$	0.345	± 0.038
$Rh(SCN)_6^{3-}$	0.428	± 0.042
TaF_8^{3-}	0.284	± 0.042
TbF_7^{3-}	0.290	± 0.038
$Tc(CN)_6^{5-}$	0.410	± 0.042
ThF_7^{3-}	0.282	± 0.042
$TiBr_6^{3-}$	0.315	± 0.038
TlF_6^{3-}	0.271	± 0.038
UF_7^{3-}	0.285	± 0.042
YF_6^{3-}	0.275	± 0.038
ZrF_7^{3-}	0.273	± 0.038
Singly Charged Cations		
$N(CH_3)_4^+$	0.234	± 0.019
$N_2H_5^+$	0.158	± 0.019
$N_2H_6^{2+}$	0.158	± 0.029
$NH(C_2H_5)_3^+$	0.274	± 0.019
$NH_3C_2H_5^+$	0.193	± 0.019
$NH_3C_3H_7^+$	0.225	± 0.019
$NH_3CH_3^+$	0.177	± 0.019
NH_3OH^+	0.147	± 0.019
NH_4^+	0.136	± 0.019
$NH_3C_2H_4OH^+$	0.203	± 0.019
$As_3S_4^+$	0.244	± 0.027
$As_3Se_4^+$	0.253	± 0.027
$AsCl_4^+$	0.221	± 0.027
Br_2^+	0.155	± 0.027
Br_3^+	0.204	± 0.027
Br_3^-	0.238	± 0.027
Br_5^+	0.229	± 0.027
$BrClCNH_2^+$	0.175	± 0.027
BrF_2^+	0.183	± 0.027
BrF_4^+	0.172	± 0.027
$C_{10}F_8^+$	0.265	± 0.027
$C_6F_6^+$	0.228	± 0.027
$Cl(SNSCN)_2^+$	0.347	± 0.027
$Cl_2C{=}NH_2^+$	0.173	± 0.027
Cl_2F^+	0.165	± 0.027
Cl_3^+	0.182	± 0.027
ClF_2^+	0.147	± 0.027
ClO_2^+	0.118	± 0.027
$GaBr_4^-$	0.317	± 0.038
I_2^+	0.185	± 0.027
I_3^+	0.225	± 0.027
I_5^+	0.263	± 0.027
IBr_2^+	0.196	± 0.027
ICl_2^+	0.175	± 0.036
IF_6^+	0.209	± 0.027
$N(S_3N_2)_2^+$	0.258	± 0.027
$N(SCl)_2^+$	0.186	± 0.027
$N(SeCl)_2^+$	0.246	± 0.027
$N(SF_2)_2^+$	0.214	± 0.027
N_2F^+	0.156	± 0.027
NO^+	0.145	± 0.027
NO_2^+	0.153	± 0.027

Ion	Radius	
O_2^+	0.140	± 0.027
$O_2(SCCF_3Cl)_2^+$	0.275	± 0.027
$ONCH_3CF_3^+$	0.200	± 0.027
$OsOF_5^-$	0.246	± 0.038
$P(CH_3)_3Cl^+$	0.197	± 0.027
$P(CH_3)_3D^+$	0.196	± 0.027
PCl_4^+	0.235	± 0.027
$ReOF_5^-$	0.245	± 0.038
$S(CH_3)_2Cl^+$	0.207	± 0.027
$S(N(C_2H_5)_3)_3^+$	0.439	± 0.027
$S_2(CH_3)_2Cl^+$	0.265	± 0.027
$S_2(CH_3)_2CN^+$	0.223	± 0.027
$S_2(CH_3)_3^+$	0.233	± 0.027
$S_2Br_5^+$	0.267	± 0.027
S_2N^+	0.159	± 0.034
$S_2N_2C_2H_3^+$	0.211	± 0.027
$S_2NC_2(PhCH_3)_2^+$	0.310	± 0.027
$S_2NC_3H_4^+$	0.218	± 0.027
$S_2NC_4H_8^+$	0.225	± 0.027
$S_3(CH_3)_3^+$	0.239	± 0.027
$S_3Br_3^+$	0.245	± 0.027
$S_3C_3H_7^+$	0.199	± 0.027
$S_3C_4F_6^+$	0.261	± 0.027
$S_3CF_3CN^+$	0.263	± 0.027
$S_3Cl_3^+$	0.233	± 0.027
$S_3N_2^+$	0.201	± 0.027
$S_3N_2Cl^+$	0.232	± 0.027
$S_4N_3^+$	0.231	± 0.027
$S_4N_3(Ph)_2^+$	0.316	± 0.027
$S_4N_4H^+$	0.178	± 0.027
$S_5N_5^+$	0.257	± 0.027
S_7I^+	0.262	± 0.027
$Sb(NPPh_3)_4^+$	0.518	± 0.027
SBr_3^+	0.220	± 0.027
$SCH_3O_2^+$	0.183	± 0.027
$SCH_3P(CH_3)_3^+$	0.248	± 0.027
$SCH_3PCH_3Cl_2^+$	0.205	± 0.027
$SCl(C_2H_5)_2^+$	0.207	± 0.027
$SCl_2CF_3^+$	0.207	± 0.027
$SCl_2CH_3^+$	0.204	± 0.027
SCl_3^+	0.185	± 0.027
$Se_3Br_3^+$	0.253	± 0.027
$Se_3Cl_3^+$	0.245	± 0.027
$Se_3N_2^+$	0.288	± 0.042
$Se_3NC_{12}^+$	0.163	± 0.027
Se_6I^+	0.260	± 0.027
$SeBr_3^+$	0.182	± 0.027
$SeCl_3^+$	0.192	± 0.027
SeF_3^+	0.179	± 0.027
SeI_3^+	0.238	± 0.027
SeN_2Cl^+	0.196	± 0.027
$SeNCl_2^+$	0.157	± 0.027
$(SeNMe_3)_3^+$	0.406	± 0.027
$SeS_2N_2^+$	0.282	± 0.042
$SF(C_6F_5)_2^+$	0.294	± 0.027
$SF_2CF_3^+$	0.198	± 0.027
$SF_2N(CH_3)_2^+$	0.210	± 0.027
SF_3^+	0.172	± 0.027
$SFS(C(CF_3)_2)_2^+$	0.275	± 0.027
$SH_2C_3H_7^+$	0.210	± 0.027
SN^+	0.158	± 0.027
$SNCl_5(CH_3CN)^-$	0.290	± 0.038
$(SNPMe_3)_3^+$	0.308	± 0.027
$SNSC(CH_3)N^+$	0.225	± 0.027
$SNSC(CN)CH^+$	0.209	± 0.027
$SNSC(Ph)N^+$	0.251	± 0.027
$SNSC(Ph)NS_3N_2^+$	0.327	± 0.027
$SNSC(PhCH_3)N^+$	0.264	± 0.027
$(Te(N(SiMe_3)_2)_2)_2^+$	0.371	± 0.027
$Te(N_3)_3^+$	0.226	± 0.027
$Te_4Nb_3OTe_2I_6^+$	0.407	± 0.027
$TeBr_3^+$	0.235	± 0.027
$TeCl_3^+$	0.216	± 0.027
$TeCl_3$(15-crown-5)$^+$	0.282	± 0.027
TeI_3^+	0.243	± 0.027
$Xe_2F_{11}^+$	0.266	± 0.027
$Xe_2F_3^+$	0.221	± 0.027
XeF^+	0.174	± 0.027
XeF_3^+	0.183	± 0.027
XeF_5^+	0.186	± 0.027
$XeOF_3^+$	0.186	± 0.027
Doubly Charged Cations		
$Co_2S_2(CO)_6^{2+}$	0.263	± 0.035
$FeW(Se)_2(CO)^{2+}$	0.260	± 0.035
I_4^{2+}	0.207	± 0.035
$Mo(Te_3)(CO)_4^{2+}$	0.234	± 0.035
S_{19}^{2+}	0.292	± 0.035
$S_2(S(CH_3)_2)_2^{2+}$	0.230	± 0.035
$S_2I_4^{2+}$	0.231	± 0.035
$S_3N_2^{2+}$	0.184	± 0.035
$S_3NCCNS_3^{2+}$	0.220	± 0.035
S_3Se^{2+}	0.326	± 0.035
$S_4N_4^{2+}$	0.186	± 0.035
$S_6N_4^{2+}$	0.232	± 0.035
S_8^{2+}	0.182	± 0.035
Se_{10}^{2+}	0.253	± 0.035
Se_{17}^{2+}	0.236	± 0.035
Se_{19}^{2+}	0.296	± 0.035
$Se_2I_4^{2+}$	0.218	± 0.035
$Se_3N_2^{2+}$	0.182	± 0.035
Se_4^{2+}	0.152	± 0.035
$Se_4S_2N_4^{2+}$	0.224	± 0.035
Se_8^{2+}	0.186	± 0.035
$SeN_2S_2^{2+}$	0.182	± 0.035
$(SNP(C_2H_5)_3)_2^{2+}$	0.312	± 0.035
$TaBr_6^-$	0.351	± 0.049
$Te(trtu)_4^{2+}$	0.328	± 0.035
$Te(tu)_4^{2+}$	0.296	± 0.035
$Te_2(esu)_4Br_2^{2+}$	0.356	± 0.035
$Te_2(esu)_4Cl_2^{2+}$	0.361	± 0.035
$Te_2(esu)_4I_2^{2+}$	0.342	± 0.035
$Te_2Se_2^{2+}$	0.192	± 0.035
$Te_2Se_4^{2+}$	0.222	± 0.035
$Te_2Se_8^{2+}$	0.252	± 0.035
$Te_3S_3^{2+}$	0.217	± 0.035
Te_3Se^{2+}	0.193	± 0.035
Te_4^{2+}	0.169	± 0.035
Te_8^{2+}	0.187	± 0.035
$W(CO)_4$(h3-Te)$^{2+}$	0.234	± 0.035
$W_2(CO)_{10}Se_4^{2+}$	0.290	± 0.035
Multi-Charged Cations		
I_{15}^{3+}	0.442	± 0.051
$Te_2(su)_6^{4+}$	0.453	± 0.034

Ligand abbreviations: su = selenourea; esu = ethyleneselenourea; tu = thiourea; ph = phenyl.

TABLE 3. Ancillary Thermochemical Data
(kJ mol^{-1})

Species	State	$\Delta_f H^o$
AsO_4^{3-}	g	(289)
BrO_3^-	g	–145
ClO_4^-	g	–344
CN^-	g	66
CO_3^{2-}	g	–321
$Fe(NO_3)_2$	c	(–448)
HF_2^-	g	–774
$HfCl_6^{2-}$	g	–1640
$IO_2F_2^-$	g	–693
IO_3^-	g	–208
$IrCl_6^{2-}$	g	–785
$LiCH_3O_2$	c	(–745)
$NbCl_6^{2-}$	g	–1224
$NH_2CH_2CO_2^-$	g	–564
O_2^{2-}	g	553
$PdCl_6^{2-}$	g	–749
PO_4^{3-}	g	291
$PtCl_6^{2-}$	g	–774
$ReBr_6^{2-}$	g	–689
$ReCl_6^{2-}$	g	–919
$Ti(OH)_2$	c	–778