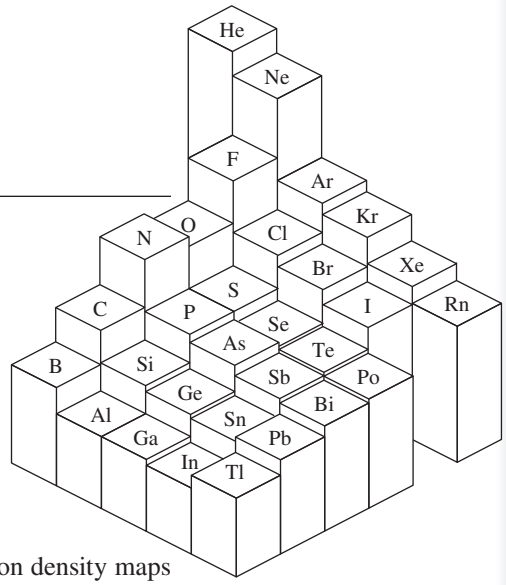
Appendix B

Useful Data



Appendix B.1: Ionic Radii

The values given are the crystal radii of Shannon, calculated using electron density maps and inter-nuclear distances from X-ray data. Some of the trends that can be seen in these radii are the following:

1. Increase in size with increasing coordination number
2. Increase in size for a given coordination number with increasing Z within a periodic group
3. Decreasing size with increasing nuclear charge for isoelectronic ions
4. Decreasing size with increasing ionic charge for the same Z
5. Irregular, slowly decreasing size with increasing Z for transition metal, lanthanide, or actinide ions of the same charge
6. Larger size for high-spin ions than for low-spin ions of the same species and charge

Not shown in the table, but another apparent factor, is the decrease in anion size with increasing cation field strength, determined by the charge and size of the cation in the crystal. (See O. Johnson, *Inorg. Chem.*, **1973**, *12*, 780, for details.)

Ionic radii are given in picometers.

		Coordination Number						
Z		2	4	6	8	10	12	14
1	H	−4						
2	(He)							
3	Li^+		60[a]	79[a]	106			
4	Be^{2+}		41	59				
5	B^{3+}		25					
6	C^{4+}		29					
7	N^{3-}		132					
8	O^{2-}	121	124	126	128			
	OH^-	118	121	123				
9	F^-	115	117	119				
10	(Ne)							
11	Na^+		113	107[a]	132		153	
12	Mg^{2+}		71	86	103			
13	Al^{3+}		53	68				
14	Si^{4+}		40	54				
15	P^{3+}			58				
16	S^{2-}			170				
17	Cl^-			167				
18	(Ar)							

(continues)

		Coordination Number						
Z		2	4	6	8	10	12	14
19	K^+		151	138[a]	165	173	178	
20	Ca^{2+}			114	126	137	148	
21	Sc^{3+}			89	101			
22	Ti^{2+}			100				
	Ti^{3+}			81				
	Ti^{4+}		56	75	88			
23	V^{2+}			93				
	V^{3+}			78				
24	Cr^{2+}			hs 94				
	Cr^{2+}			ls 87				
	Cr^{3+}			76				
25	Mn^{2+}		hs 80	hs 97				
	Mn^{2+}			ls 81				
	Mn^{3+}			hs 79				
	Mn^{3+}			ls 72				
26	Fe^{2+}		hs 77	hs 92				
	Fe^{2+}			ls 75				
	Fe^{3+}		hs 63	hs 79				
	Fe^{3+}			ls 69				
27	Co^{2+}		hs 72	hs 89				
	Co^{2+}			ls 79				
	Co^{3+}			hs 75				
	Co^{3+}			ls 69				
28	Ni^{2+}		69	83				
	Ni^{2+}		sq 63					
	Ni^{3+}			hs 74				
	Ni^{3+}			ls 70				
29	Cu^+	60	74	91				
	Cu^{2+}		71	87				
30	Zn^{2+}		74	88	104			
31	Ga^{3+}		61	76				
32	Ge^{4+}		53	67				
33	As^{3+}			72				
	As^{5+}		48	60				
34	Se^{2-}			184				
35	Br^-			182				
36	(Kr)							
37	Rb^+			166	164[a]	180	186	197
38	Sr^{2+}			132	140	150	158	
39	Y^{2+}			104				
40	Zr^{4+}		73	86	98			
41	Nb^{3+}			86				
	Nb^{4+}			82	93			
42	Mo^{3+}			83				
	Mo^{4+}			79				
43	Tc^{4+}			79				
44	Ru^{3+}			82				
	Ru^{4+}			76				
45	Rh^{3+}			81				
	Rh^{4+}			74				
46	Pd^{2+}		sq 78	100				
47	Ag^+	81	114	129	142			

(continues)

		Coordination Number						
Z		2	4	6	8	10	12	14
	Ag^{+}		sq 116					
48	Cd^{2+}		92	109	124		145	
49	In^{3+}		76	94	106			
50	Sn^{4+}		69	83	95			
51	Sb^{3+}			90				
52	Te^{2-}			207				
53	I^{-}			206				
54	(Xe)							
55	Cs^{+}			181	173[a]	195	202	
56	Ba^{2+}			149	156	166	175	
57	La^{3+}			117	130	141	150	
58	Ce^{3+}			115	128	139	148	
59	Pr^{3+}			113	127			
60	Nd^{3+}			112	125		141	
61	Pm^{3+}			111	123			
62	Sm^{3+}			110	122		138	
63	Eu^{3+}			109	121			
64	Gd^{3+}			108	119			
65	Tb^{3+}			106	118			
66	Dy^{3+}			105	117			
67	Ho^{3+}			104	116	126		
68	Er^{3+}			103	114			
69	Tm^{3+}			102	113			
70	Yb^{3+}			101	113			
71	Lu^{3+}			100	112			
72	Hf^{4+}		72	85	97			
73	Ta^{3+}			86				
	Ta^{4+}			82				
74	W^{4+}			80				
75	Re^{4+}			77				
76	Os^{4+}			77				
77	Ir^{3+}			82				
	Ir^{4+}			77				
78	Pt^{2+}		sq 74	94				
	Pt^{4+}			77				
79	Au^{+}			151				
	Au^{3+}		sq 82	99				
80	Hg^{2+}	83	110	116	128			
81	Tl^{3+}		89	103	112			
82	Pb^{2+}		112	133	143	154	163	
	Pb^{4+}		79	92	108			
83	Bi^{3+}			117	131			
84	Po^{4+}			108	122			
85	At^{7+}			76				
86	(Rn)							
87	Fr^{+}			194				
88	Ra^{2+}				162		184	
89	Ac^{3+}			126				
90	Th^{4+}			108	119	127	135	

Most values from R. D. Shannon, *Acta Crystallogr.*, **1976**, *A32*, 751.

[a]Proposed values from J. Mähler, I. Persson, *Inorg. Chem.*, **2012**, *51*, 425.

hs = high spin, ls = low spin, sq = square planar; values for CN = 4 are for tetrahedral geometry unless designated square planar.

Appendix B.2: Ionization Energy

Atomic No.	Element	eV	kJ mol^{-1}	Atomic No.	Element	eV	kJ mol^{-1}
1	H	13.598	1,312.0	52	Te	9.009	869.2
2	He	24.587	2,372.8	53	I	10.451	1,008.4
3	Li	5.392	520.2	54	Xe	12.130	1,170.4
4	Be	9.322	899.4	55	Cs	3.894	375.7
5	B	8.298	800.6	56	Ba	5.212	502.9
6	C	11.260	1,086.5	57	La	5.577	538.1
7	N	14.534	1,402.3	58	Ce	5.47	528
8	O	13.618	1,314.0	59	Pr	5.42	523
9	F	17.422	1,681.0	60	Nd	5.49	530
10	Ne	21.564	2,080.6	61	Pm	5.55	535
11	Na	5.139	495.8	62	Sm	5.63	543
12	Mg	7.646	737.8	63	Eu	5.67	547
13	Al	5.986	577.6	64	Gd	6.14	592
14	Si	8.151	786.5	65	Tb	5.85	564
15	P	10.486	1,011.7	66	Dy	5.93	572
16	S	10.360	999.6	67	Ho	6.02	581
17	Cl	12.967	1,251.1	68	Er	6.10	589
18	Ar	15.759	1,520.5	69	Tm	6.18	596
19	K	4.341	418.8	70	Yb	6.254	603.4
20	Ca	6.113	589.8	71	Lu	5.426	523.5
21	Sc	6.54	631	72	Hf	7.0	675
22	Ti	6.82	658	73	Ta	7.89	761
23	V	6.74	650	74	W	7.98	770
24	Cr	6.766	652.8	75	Re	7.88	760
25	Mn	7.435	717.4	76	Os	8.7	839
26	Fe	7.870	759.3	77	Ir	9.1	878
27	Co	7.86	758	78	Pt	9.0	868
28	Ni	7.635	736.7	79	Au	9.225	890.1
29	Cu	7.726	745.5	80	Hg	10.437	1,007.0
30	Zn	9.394	906.4	81	Tl	6.108	589.3
31	Ga	5.999	578.8	82	Pb	7.416	715.5
32	Ge	7.899	762.1	83	Bi	7.289	703.3
33	As	9.81	947	84	Po	8.42	812
34	Se	9.752	940.9	85	At	7.289	703.3
35	Br	11.814	1,139.9	86	Rn	10.748	1,037.1
36	Kr	13.999	1,350.7	87	Fr	4	400
37	Rb	4.177	403.0	88	Ra	5.279	509.3
38	Sr	5.695	549.5	89	Ac	6.9	666
39	Y	6.38	616	90	Th	6.1	590
40	Zr	6.84	660	91	Pa	5.9	570
41	Nb	6.88	664	92	U	6.1	590
42	Mo	7.099	684.9	93	Np	6.2	600
43	Tc	7.28	702	94	Pu	6.06	585
44	Ru	7.37	711	95	Am	5.99	578
45	Rh	7.46	720	96	Cm	6.02	581
46	Pd	8.34	805	97	Bk	6.23	601
47	Ag	7.576	731.0	98	Cf	6.30	608
48	Cd	8.993	867.7	99	Es	6.42	619
49	In	5.786	558.3	100	Fm	6.50	627
50	Sn	7.344	708.6	101	Md	6.58	635
51	Sb	8.641	833.7	102	No	6.65	642

Source: C. E. Moore, *Ionization Potentials and Limits Derived from the Analyses of Optical Spectra*, NSRDS-NBS 34, National Bureau of Standards, Washington, DC, 1970; W. C. Martin, L. Hagan, J. Reador, J. Sugar, *J. Phys. Chem. Ref. Data*, **1974**, *3*, 771; and J. Sugar, *J. Opt. Soc. Am.*, **1975**, *65*, 1366.

NOTE: 1 eV = 96.4853 kJ mol^{-1}.

Ionization energies are available at webbook.nist.gov/chemistry

Appendix B.3: Electron Affinity

Atomic No.	Element	eV	kJ mol^{-1}	Atomic No.	Element	eV	kJ mol^{-1}
1	H	0.754	72.8	45	Rh	1.137	109.7
2	He	−0.5*	−50	46	Pd	0.557	53.7
3	Li	0.618	59.6	47	Ag	1.302	125.6
4	Be	−0.5*	−50	48	Cd	−0.7*	−68
5	B	0.277	26.7	49	In	0.3	29
6	C	1.263	121.9	50	Sn	1.2	116
7	N	−0.07	−7	51	Sb	1.07	103
8	O	1.461	141.0	52	Te	1.971	190.2
9	F	3.399	328.0	53	I	3.059	295.2
10	Ne	−1.2*	−116	54	Xe	−0.8*	−77
11	Na	0.548	52.9	55	Cs	0.472	45.5
12	Mg	−0.4*	−39	56	Ba	−0.3*	−29
13	Al	0.441	42.6	57	La	0.5	48
14	Si	1.385	133.6	58	Ce	<0.5[a]	<48
15	P	0.747	72.0	59	Pr	<0.5[a]	<48
16	S	2.077	200.4	60	Nd	<0.5[a]	<48
17	Cl	3.617	349.0	61	Pm	<0.5[a]	<48
18	Ar	−1.0*	−97	62	Sm	<0.5[a]	<48
19	K	0.501	48.4	63	Eu	<0.5[a]	<48
20	Ca	−0.3*	−29	64	Gd	<0.5[a]	<48
21	Sc	0.188	18.1	65	Tb	<0.5[a]	<48
22	Ti	0.079	7.6	66	Dy	<0.5[a]	<48
23	V	0.525	50.7	67	Ho	<0.5[a]	<48
24	Cr	0.666	64.3	68	Er	<0.5[a]	<48
25	Mn	<0	<0.0	69	Tm	<0.5[a]	<48
26	Fe	0.163	15.7	70	Yb	<0.5[a]	<48
27	Co	0.661	63.8	71	Lu	<0.5[a]	<48
28	Ni	1.156	111.5	72	Hf	~0	~0
29	Cu	1.228	118.5	73	Ta	0.322	31.1
30	Zn	−0.6*	−58	74	W	0.815	78.6
31	Ga	0.3	29	75	Re	0.15	14.5
32	Ge	1.2	115.8	76	Os	1.1	106.1
33	As	0.81	78	77	Ir	1.565	151.0
34	Se	2.021	195.0	78	Pt	2.128	205.3
35	Br	3.365	324.7	79	Au	2.309	222.8
36	Kr	−1.0*	−97	80	Hg	−0.5*	−48
37	Rb	0.486	46.9	81	Tl	0.2	19
38	Sr	−0.3*	−29	82	Pb	0.364	35.1
39	Y	0.307	29.6	83	Bi	0.946	91.3
40	Zr	0.426	41.1	84	Po	1.9	183
41	Nb	0.893	86.2	85	At	2.8	270
42	Mo	0.746	72.0	86	Rn	−0.7*	−68
43	Tc	0.55	53.1	87	Fr	0.6*	58
44	Ru	1.05	101.3	88	Ra	−0.3*	−29

All data from W. Hotop, W. C. Lineberger, *J. Phys. Chem. Ref. Data*, **1985**, *14*, 731, except those marked*, which are from S. G. Bratsch, J. J. Lagowski, *Polyhedron*, **1986**, 5, 1763.

Many of these data are known to greater accuracy than that shown in the table, some to 10 significant figures. Updated electron affinities can be found at webbook.nist.gov.

[a] Estimated values

Appendix B.4: Electronegativity[a]

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 2.300																	He 4.160
Li 0.912	Be 1.576											B 2.051	C 2.544	N 3.066	O 3.610	F 4.193	Ne 4.787
Na 0.869	Mg 1.293											Al 1.613	Si 1.916	P 2.253	S 2.589	Cl 2.869	Ar 3.242
K 0.734	Ca 1.034	Sc 1.19	Ti 1.38	V 1.53	Cr 1.65	Mn 1.75	Fe 1.80	Co 1.84	Ni 1.88	Cu 1.85	Zn 1.588	Ga 1.756	Ge 1.994	As 2.211	Se 2.424	Br 2.685	Kr 2.966
Rb 0.706	Sr 0.963	Y 1.12	Zr 1.32	Nb 1.41	Mo 1.47	Tc 1.51	Ru 1.54	Rh 1.56	Pd 1.58	Ag 1.87	Cd 1.521	In 1.656	Sn 1.824	Sb 1.984	Te 2.158	I 2.359	Xe 2.582
Cs 0.659	Ba 0.881	Lu 1.09	Hf 1.16	Ta 1.34	W 1.47	Re 1.60	Os 1.65	Ir 1.68	Pt 1.72	Au 1.92	Hg 1.765	Tl 1.789	Pb 1.854	Bi (2.01)	Po (2.19)	At (2.39)	Rn (2.60)

J. B. Mann, T. L. Meek, L. C. Allen, *J. Am. Chem. Soc.*, **2000**, *122*, 2780, and J. B. Mann, T. L. Meek, E. T. Knight, J. F. Capitani, L. C. Allen, *J. Am. Chem. Soc.*, **2000**, *122*, 5132.

[a]The shaded elements are metalloids, on the basis of their electronegativities.

Appendix B.5: Absolute Hardness Parameters

Hardness Parameters (in eV)					
	Ion or Molecule	I	A	χ	η
Cations	B^{3+}	259.37	37.93	148.65	110.72
	Be^{2+}	153.89	18.21	86.05	67.84
	Al^{3+}	119.99	28.45	74.22	45.77
	Li^{+}	75.64	5.39	40.52	35.12
	Mg^{2+}	80.14	15.04	47.59	32.55
	Na^{+}	47.29	5.14	26.21	21.08
	Ca^{2+}	50.91	11.87	31.39	19.52
	Sr^{2+}	43.6	11.03	27.3	16.3
	K^{+}	31.63	4.34	17.99	13.64
	Fe^{3+}	54.8	30.65	42.73	12.08
	Rb^{+}	27.28	4.18	15.77	11.55
	Rh^{3+}	53.4	31.1	42.4	11.2
	Zn^{2+}	39.72	17.96	28.84	10.88
	Cs^{+}	25.1	3.89	14.5	10.6
	Cd^{2+}	37.48	16.91	27.20	10.29
	Cr^{3+}	49.1	30.96	40.0	9.1
	Mn^{2+}	33.67	15.64	24.66	9.02
	Mn^{3+}	51.2	33.67	42.4	8.8
	Co^{3+}	51.3	33.50	42.4	8.9
	V^{3+}	46.71	29.31	38.01	8.70

(continues)

Hardness Parameters (in eV)					
	Ion or Molecule	I	A	χ	η
	Ni^{2+}	35.17	18.17	26.67	8.50
	Pb^{2+}	31.94	15.03	23.49	8.46
	Au^{3+}	54.1	37.4	45.8	8.4
	Cu^{2+}	36.83	20.29	28.56	8.27
	Co^{2+}	33.50	17.06	25.28	8.22
	Pt^{2+}	35.2	19.2	27.2	8.0
	Sn^{2+}	30.50	14.63	22.57	7.94
	Ir^{3+}	45.3	29.5	37.4	7.9
	Hg^{2+}	34.2	18.76	26.5	7.7
	V^{2+}	29.31	14.65	21.98	7.33
	Fe^{2+}	30.65	16.18	23.42	7.24
	Cr^{2+}	30.96	16.50	23.73	7.23
	Ag^{+}	21.49	7.58	14.53	6.96
	Ti^{2+}	27.49	13.58	20.54	6.96
	Pd^{2+}	32.93	19.43	26.18	6.75
	Rh^{2+}	31.06	18.08	24.57	6.49
	Cu^{+}	20.29	7.73	14.01	6.28
	Sc^{2+}	24.76	12.80	18.78	5.98
	Ru^{2+}	28.47	16.76	22.62	5.86
	Au^{+}	20.5	9.23	14.90	5.6
Molecules	BF_3	15.81	–3.5	6.2	9.7
	H_2O	12.6	–6.4	3.1	9.5
	N_2	15.58	–2.2	6.70	8.9
	NH_3	10.7	–5.6	2.6	8.2
	CH_3CN	12.2	–2.8	4.7	7.5
	C_2H_2	11.4	–2.6	4.4	7.0
	PF_3	12.3	–1.0	5.7	6.7
	$(CH_3)_3N$	7.8	–4.8	1.5	6.3
	C_2H_4	10.5	–1.8	4.4	6.2
	PH_3	10.0	–1.9	4.1	6.0
	O_2	12.2	0.4	6.3	5.9
	$(CH_3)_3P$	8.6	–3.1	2.8	5.9
	$(CH_3)_3As$	8.7	–2.7	3.0	5.7
	SO_2	12.3	1.1	6.7	5.6
	SO_3	12.7	1.7	7.2	5.5
	C_6H_6	9.3	–1.2	4.1	5.3
	C_5H_5N	9.3	–0.6	4.4	5.0
	Butadiene	9.1	–0.6	4.3	4.9
	PCl_3	10.2	0.8	5.5	4.7
	PBr_3	9.9	1.6	5.6	4.2

Hardness Parameters for Atoms and Radicals (in eV)[a]				
Atom or Radical	I	A	χ	η
F	17.42	3.40	10.41	7.01
H	13.60	0.75	7.18	6.43
OH	13.17	1.83	7.50	5.67
NH_2	11.40	0.74	6.07	5.33
CN	14.02	3.82	8.92	5.10
CH_3	9.82	0.08	4.96	4.87
Cl	13.01	3.62	8.31	4.70
C_2H_5	8.38	− 0.39	4.00	4.39
Br	11.81	3.36	7.60	4.24
C_6H_5	9.20	1.1	5.2	4.1
NO_2	>10.1	2.30	>6.2	>3.9
I	10.45	3.06	6.76	3.70
SiH_3	8.14	1.41	4.78	3.37
C_6H_5O	8.85	2.35	5.60	3.25
$Mn(CO)_5$	8.44	2.0	5.2	3.2
CH_3S	8.06	1.9	5.0	3.1
C_6H_5S	8.63	2.47	5.50	3.08

(Created using data from R. G. Pearson, *Inorg. Chem.*, 27, 1988, 734.)
[a]The hardness values approximate those of the corresponding anions.

Appendix B.6: C_A, E_A, C_B, and E_B Values

Acid	C_A	E_A
Trimethylboron, $B(CH_3)_3$	1.70	6.14
Boron trifluoride (gas), BF_3	1.62	9.88
Trimethylaluminum, $Al(CH_3)_3$	1.43	16.9
Iodine (standard), I_2	1.00[a]	1.00[a]
Trimethylgallium, $Ga(CH_3)_3$	0.881	13.3
Iodine monochloride, ICl	0.830	5.10
Sulfur dioxide, SO_2	0.808	0.920
Phenol, C_6H_5OH	0.442	4.33
tert-Butyl alcohol, C_4H_9OH	0.300	2.04
Pyrrole, C_4H_4NH	0.295	2.54
Chloroform, $CHCl_3$	0.159	3.02

(continues)

Base	C_B	E_B
1-Azabicyclo[2.2.2] octane, (quinuclidine)	13.2	0.704
Trimethylamine, $(CH_3)_3N$	11.54	0.808
Triethylamine, $(C_2H_5)_3N$	11.09	0.991
Dimethylamine, $(CH_3)_2NH$	8.73	1.09
Diethyl sulfide, $(C_2H_5)_2S$	7.40[a]	0.339
Pyridine, C_5H_5N	6.40	1.17
Methylamine, CH_3NH_2	5.88	1.30
Pyridine-N-oxide, C_5H_5NO	4.52	1.34
Tetrahydrofuran, C_4H_8O	4.27	0.978
7-Oxabicyclo[2.2.1] heptane, $C_6H_{10}O$	3.76	1.08
Ammonia, NH_3	3.46	1.36
Diethyl ether, $(C_2H_5)_2O$	3.25	0.963
Dimethyl sulfoxide, $(CH_3)_2SO$	2.85	1.34
N,N-dimethylacetamide, $(CH_3)_2NCOCH_3$	2.58	1.32[a]
p-Dioxane, $O(C_2H_4)_2O$	2.38	1.09
Acetone, CH_3COCH_3	2.33	0.987
Acetonitrile, CH_3CN	1.34	0.886
Benzene, C_6H_6	0.681	0.525

[a] Reference values.

(Created using data from R. S. Drago, *J. Chem. Educ.*, 51, 1974, 300.)

Appendix B.7: Latimer Diagrams For Selected Elements[1]

ACIDIC SOLUTION

$$H^+ \xrightarrow{0} H_2 \xrightarrow{-2.25} H^-$$

Group 1

$$Li^+ \xrightarrow{-3.04} Li \quad Na^+ \xrightarrow{-2.71} Na \quad K^+ \xrightarrow{-2.92} K \quad Rb^+ \xrightarrow{-2.92} Rb \quad Cs^+ \xrightarrow{-2.92} Cs$$

Group 2

$$Be^{2+} \xrightarrow{-1.97} Be \quad Mg^{2+} \xrightarrow{-2.36} Mg \quad Ca^{2+} \xrightarrow{-2.84} Ca \quad Sr^{2+} \xrightarrow{-2.89} Sr \quad Ba^{2+} \xrightarrow{-2.92} Ba$$

[1]Data from A. J. Bard, R. Parsons, and J. Jordan, eds., *Standard Potentials in Aqueous Solution*, Marcel Dekker, New York, 1985; A. Kaczmarcyzk, W. C. Nichols, W. H. Stockmayer, T. B. Ames, *Inorg. Chem.*, **1968**, *7*, 1057; M. Pourbaix, *Atlas of Electrochemical Equilibria in Aqueous Solution,* 2d ed., translated by J. A. Franklin, National Association of Corrosion Engineers, Houston, TX, 1974.

Group 3

$$Sc^{3+} \xrightarrow{-2.03} Sc \quad Y^{3+} \xrightarrow{-2.37} Y \quad La^{3+} \xrightarrow{-2.38} La \quad Ac^{3+} \xrightarrow{-2.13} Ac$$

Group 4

$$TiO^{2+} \xrightarrow{0.10} Ti^{3+} \xrightarrow{-0.37} Ti^{2+} \xrightarrow{-1.63} Ti$$

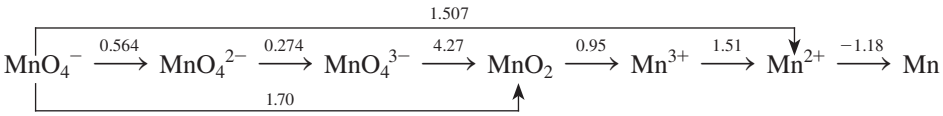
Group 5

$$V(OH)_4^{+} \xrightarrow{1.00} VO^{2+} \xrightarrow{0.34} V^{3+} \xrightarrow{-0.26} V^{2+} \xrightarrow{-1.13} V$$

Group 6

$$Cr_2O_7^{2-} \xrightarrow{1.38} Cr^{3+} \xrightarrow{-0.42} Cr^{2+} \xrightarrow{-0.90} Cr$$

Group 7



Group 8

$$FeO_4^{2-} \xrightarrow{2.20} Fe^{3+} \xrightarrow{0.771} Fe^{2+} \xrightarrow{-0.44} Fe$$

Group 9

$$CoO_2 \xrightarrow{1.416} Co^{3+} \xrightarrow{1.92} Co^{2+} \xrightarrow{-0.277} Co$$

Group 10

$$NiO_4^{2-} \xrightarrow{>1.8} NiO_2 \xrightarrow{1.59} Ni^{2+} \xrightarrow{-0.257} Ni$$
$$\text{>1.6}$$

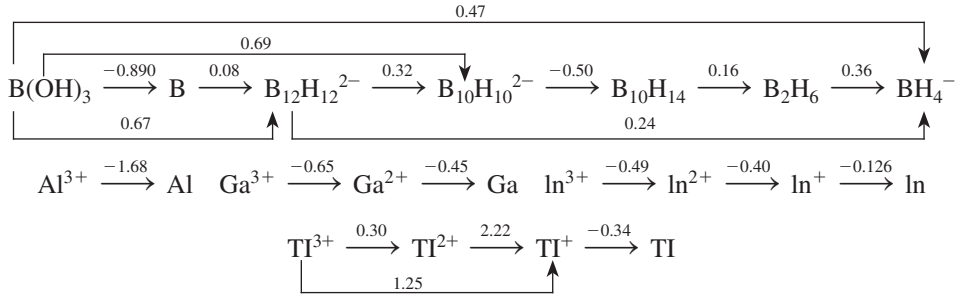
Group 11

$$CuO^{2+} \xrightarrow{1.8} Cu^{2+} \xrightarrow{0.159} Cu^{+} \xrightarrow{0.521} Cu$$
$$0.340$$

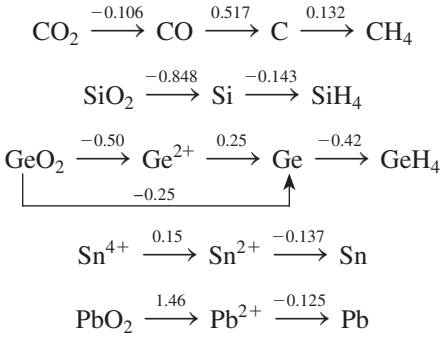
Group 12

$$Zn^{2+} \xrightarrow{-0.763} Zn \quad Cd^{2+} \xrightarrow{-0.403} Cd \quad Hg^{2+} \xrightarrow{0.911} Hg_2^{2+} \xrightarrow{0.796} Hg$$

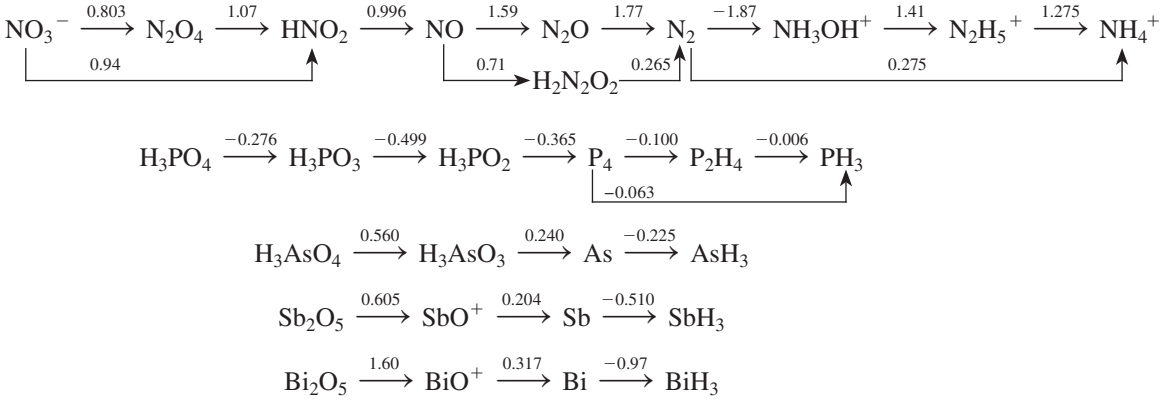
Group 13



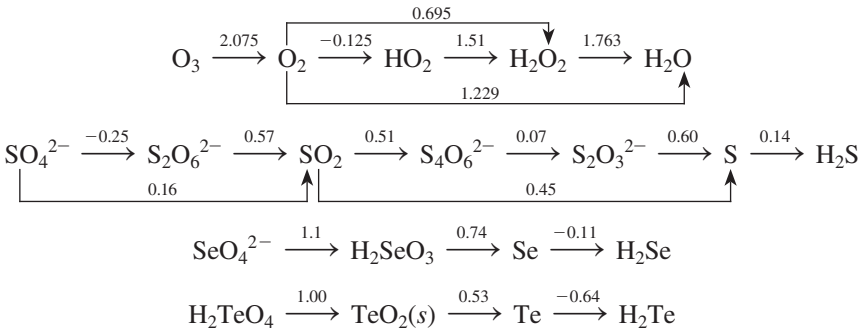
Group 14



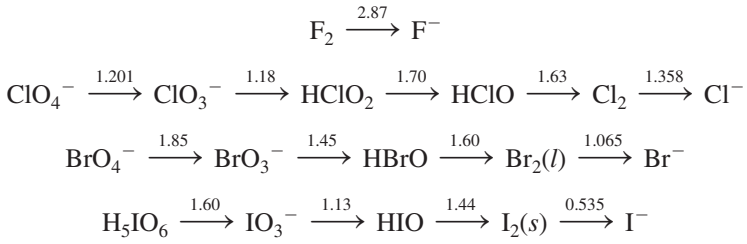
Group 15



Group 16

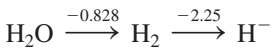


Group 17

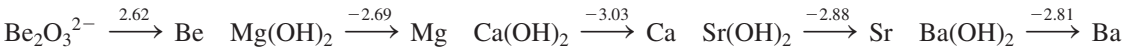


BASIC SOLUTION

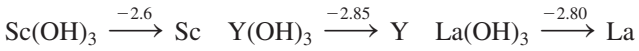
Group 1



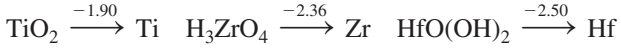
Group 2



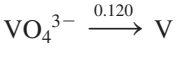
Group 3



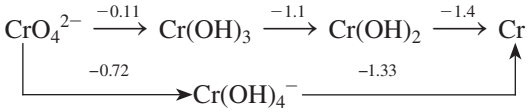
Group 4



Group 5

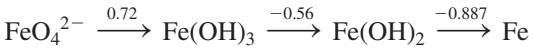


Group 6

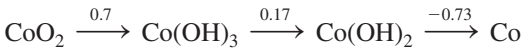


Group 7

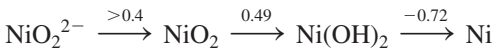
Group 8



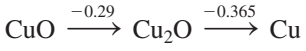
Group 9



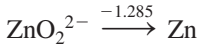
Group 10



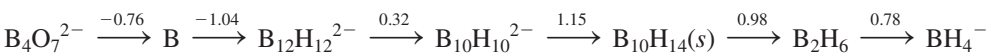
Group 11

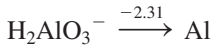


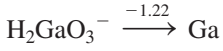
Group 12

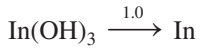


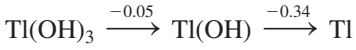
Group 13











Group 14

$$CO_3^{2-} \xrightarrow{-1.01} HCO_2^- \xrightarrow{-0.52} C \xrightarrow{-0.70} CH_4$$

$$SiO_3^{2-} \xrightarrow{-1.69} Si \xrightarrow{-0.93} SiH_4$$

$$HGeO_3^- \xrightarrow{-0.89} Ge \xrightarrow{<-1.1} GeH_4$$

$$Sn(OH)_6^{2-} \xrightarrow{-0.90} HSnO_2^- \xrightarrow{-0.91} Sn$$

$$PbO_2 \xrightarrow{0.25} PbO \xrightarrow{-0.58} Pb$$

Group 15

$$NO_3^- \xrightarrow{-0.86} N_2O_4 \xrightarrow{0.867} NO_2^- \xrightarrow{-0.46} NO \xrightarrow{0.76} N_2O \xrightarrow{0.94} N_2 \xrightarrow{-3.04} NH_2OH \xrightarrow{0.73} N_2H_4 \xrightarrow{0.1} NH_3$$

$$PO_4^{3-} \xrightarrow{-1.12} HPO_3^{2-} \xrightarrow{-1.57} H_2PO_2^- \xrightarrow{-2.05} P_4 \xrightarrow{-0.89} PH_3$$

$$AsO_4^{3-} \xrightarrow{-0.67} H_2AsO_3^- \xrightarrow{-0.68} As \xrightarrow{-1.37} AsH_3$$

$$Sb(OH)_6^- \xrightarrow{-0.465} SbO_2^- \xrightarrow{-0.639} Sb \xrightarrow{-1.34} SbH_3$$

$$Bi_2O_5 \xrightarrow{0.78} Bi_2O_4 \xrightarrow{0.56} Bi_2O_3 \xrightarrow{-0.46} Bi \xrightarrow{<-1.6} BiH_3$$

Group 16

$$O_3 \xrightarrow{2.075} O_2 \xrightarrow{-0.069} HO_2^- \xrightarrow{0.867} OH^-$$

$$SO_4^{2-} \xrightarrow{-0.94} SO_3^{2-} \xrightarrow{-0.79} S_4O_6^{2-} \xrightarrow{0.08} S_2O_3^{2-} \xrightarrow{-0.74} S \xrightarrow{-0.45} S^{2-}$$

$$SO_3^{2-} \xrightarrow{-0.66} S$$

$$SeO_4^{2-} \xrightarrow{0.03} SeO_3^{2-} \xrightarrow{-0.36} Se \xrightarrow{-0.67} Se^{2-}$$

$$TeO_2(OH)_4^{2-} \xrightarrow{0.07} TeO_3^{2-} \xrightarrow{-0.42} Te \xrightarrow{-1.14} Te^{2-}$$

Group 17

$$F_2 \xrightarrow{2.87} F^-$$

$$ClO_4^- \xrightarrow{0.374} ClO_3^- \xrightarrow{-0.48} ClO_2 \xrightarrow{1.07} ClO_2^- \xrightarrow{0.681} ClO^- \xrightarrow{0.421} Cl_2 \xrightarrow{1.358} Cl^-$$

$$ClO_3^- \xrightarrow{0.295} ClO_2^-$$

$$BrO_4^- \xrightarrow{1.025} BrO_3^- \xrightarrow{0.49} BrO^- \xrightarrow{0.455} Br_2(l) \xrightarrow{1.065} Br^-$$

$$H_3IO_6^{2-} \xrightarrow{0.65} IO_3^- \xrightarrow{0.15} IO^- \xrightarrow{0.42} I_2(s) \xrightarrow{0.535} I^-$$

Group 18

$$HXeO_6^{3-} \xrightarrow{0.94} HXeO_4^- \xrightarrow{1.24} Xe$$

Appendix B.8: Angular Functions for Hydrogen Atom *f* Orbitals

There is no unique set of angular functions for *f* orbitals. The most commonly used sets are provided here.

Cubic Set:

Orbital	Angular Function $\Theta\Phi$ (x, y, z)
f_{x^3}	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\,x(5x^2 - 3r^2)/r^3$
f_{y^3}	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\,y(5y^2 - 3r^2)/r^3$
f_{z^3}	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\,z(5z^2 - 3r^2)/r^3$
$f_{x(z^2-y^2)}$	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,x(z^2 - y^2)/r^3$
$f_{y(z^2-x^2)}$	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,y(z^2 - x^2)/r^3$
$f_{z(x^2-y^2)}$	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,z(x^2 - y^2)/r^3$
f_{xyz}	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,xyz/r^3$

General Set:

Orbital	Angular Function $\Theta\Phi$ (x, y, z)
f_{z^3}	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\,z(5z^2 - 3r^2)/r^3$
f_{xz^2}	$\frac{1}{8}\sqrt{\frac{42}{\pi}}\,x(5z^2 - r^2)/r^3$
f_{yz^2}	$\frac{1}{8}\sqrt{\frac{42}{\pi}}\,y(5z^2 - r^2)/r^3$
$f_{y(3x^2-y^2)}$	$\frac{1}{8}\sqrt{\frac{70}{\pi}}\,y(3x^2 - y^2)/r^3$
$f_{x(x^2-3y^2)}$	$\frac{1}{8}\sqrt{\frac{70}{\pi}}\,x(x^2 - 3y^2)/r^3$
f_{xyz}	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,xyz/r^3$
$f_{z(x^2-y^2)}$	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\,z(x^2 - y^2)/r^3$

Appendix B.9: Orbital Potential Energies

Atomic Number	Element	Potential Energy (eV)	
		1*s*	
1	H	–13.61	
2	He	–24.59	
		2*s*	**2*p***
3	Li	–5.39	
4	Be	–9.32	
5	B	–14.05	–8.30
6	C	–19.43	–10.66
7	N	–25.56	–13.18
8	O	–32.38	–15.85
9	F	–40.17	–18.65
10	Ne	–48.47	–21.59
		3*s*	**3*p***
11	Na	–5.14	
12	Mg	–7.65	
13	Al	–11.32	–5.98
14	Si	–14.89	–7.78
15	P	–18.84	–9.65
16	S	–22.71	–11.62
17	Cl	–25.23	–13.67
18	Ar	–29.24	–15.82
		4*s*	**4*p***
19	K	–4.34	
20	Ca	–6.11	
		4*s*	**3*d***
21	Sc	–6.60	–7.92
22	Ti	–7.12	–9.22
23	V	–7.32	–10.11
24	Cr	–7.46	–10.75
25	Mn	–7.84	–11.14
26	Fe	–7.91	–11.66
27	Co	–8.10	–12.12
28	Ni	–8.22	–12.93
29	Cu	–8.42	–13.47
30	Zn	–9.39	–17.30
		4*s*	**4*p***
31	Ga	–12.61	–5.93
32	Ge	–16.05	–7.54
33	As	–18.94	–9.17
34	Se	–21.37	–10.82
35	Br	–24.37	–12.49
36	Kr	–27.51	–14.22

(continues)

Atomic Number	Element	Potential Energy (eV)	
		5s	***5p***
37	Rb	–4.18	
38	Sr	–5.70	
		5s	***4d***
39	Y	–6.70	–6.49
40	Zr	–7.31	–8.31
41	Nb	–7.22	–8.86
42	Mo	–7.24	–9.14
43	Tc	–7.21	–9.25
44	Ru	–7.13	–9.31
45	Rh	–7.28	–9.45
46	Pd	–7.44	–9.58
47	Ag	–7.58	–12.78
48	Cd	–8.99	–17.84
		5s	***5p***
49	In	–11.89	–5.60
50	Sn	–14.56	–7.01
51	Sb	–16.74	–8.41
52	Te	–18.71	–9.79
53	I	–20.89	–11.18
54	Xe	–23.40	–12.56
		6s	***6p***
55	Cs	–3.90	
56	Ba	–5.21	
		6s	***5d***
71	Lu	–7.04	–5.28
72	Hf	–7.52	–6.14
73	Ta	–8.45	–7.58
74	W	–8.52	–8.76
75	Re	–8.76	–9.70
76	Os	–8.82	–10.00
77	Ir	–8.83	–10.22
78	Pt	–8.75	–10.37
79	Au	–9.22	–11.86
80	Hg	–10.44	–15.59
		6s	***6p***
81	Tl	–13.14	–5.47
82	Pb	–15.12	–6.81
83	Bi	(–17.52)	–8.15
84	Po	(–20.05)	(–9.42)
85	At	(–22.69)	(–10.71)
86	Rn	(–25.47)	–12.03

J. B. Mann, T. L. Meek, L. C. Allen, *J. Am. Chem. Soc.*, **2000**, *122*, 2780 and J. B. Mann, T. L. Meek, E. T. Knight, J. F. Capitani, L. C. Allen, *J. Am. Chem. Soc.*, **2000**, *122*, 5132.