Data for General, Organic, and Physical Chemistry

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Table 1. The Elements: Symbols, Atomic Numbers (Z), Atomic Weights (At. Wt), and Pauling Electronegativities (c)

Element	Symbol	Z	Atomic Weight	χ
Actinium	Ac	89	(227)	1.1
Aluminum	Al	13	26.9815	1.5
Americium	Am	95	(243)	1.3
Antimony	Sb	51	121.75	1.9
Argon	Ar	18	39.948	
Arsenic	As	33	74.9216	2.0
Astatine	At	85	(210)	2.2
Barium	Ba	56	137.	0.9
Berkelium	Bk	97	(247)	1.3
Beryllium	Be	4	9.0122	1.5
Bismuth	Bi	83	208.980	1.9
Boron	B	5	10.81	2.0
Bromine	Br	35	79.904	2.8
Cadmium	Cd	48	112.40	1.7
Calcium	Ca	20	40.08	1.0
Californium	Cf	98	(251)	1.3
Carbon	C	6	12.011	2.5
Cerium	Ce	58	140.12	1.1
Cesium	Cs	55	132.9054	0.7
Chlorine	Cl	17	35.453	3.0
Chromium	Cr	24	51.996	1.6
Cobalt	Co	27	58.9332	1.8
Copper	Cu	29	63.546	1.9
Curium	Cm	96	(247)	1.3
Dysprosium	Dy	66	162.50	1.1
Einsteinium	Es	99	(254)	1.3
Erbium	Er	68	167.26	1.1
Europium	Eu	63	151.96	1.1
Fermium	Fm	100	(257)	1.3
Fluorine	F	9	18.9984	4.0
Francium	Fr	87	(223)	0.7
Gadolinium	Gd	64	157.25	1.1
Gallium	Ga	31	69.72	1.6
Germanium	Ge	32	72.59	1.8
Gold	Au	79	196.966	2.4
Hafnium	Hf	72	178.49	1.3
Helium	He	2	4.00260	
Holmium	Ho	67	164.930	1.1
Hydrogen	H	1	1.0079	2.1
Indium	In	49	114.82	1.7
Iodine	I	53	126.904	2.5
Iridium	Ir	77	192.22	2.2
Iron	Fe	26	55.847	1.8
Krypton	Kr	36	83.80	
Lanthanum	La	57	138.905	1.1
Lawrencium	Lr	103	(256)	
Lead	Pb	82	207.2	1.8
Lithium	Li	3	6.941	1.0
Lutetium	Lu	71	174.97	1.2
Magnesium	Mg	12	24.305	1.2
Manganese	Mn	25	54.9380	1.5
Mendelevium	Md	101	(258)	1.3
Mercury	Hg	80	200.59	1.9
Molybdenum	Mo	42	95.94	1.8
Neodymium	Nd	60	144.24	1.1
Neon	Ne	10	20.179	
Neptunium	Np	93	237.048	1.3
Nickel	Ni	28	58.70	1.8
Niobium	Nb	41	92.9064	1.6
Nitrogen	N	7	14.0067	3.0
Nobelium	No	102	(255)	1.3
Osmium	Os	76	190.2	2.2
Oxygen	O	8	15.9994	3.5
Palladium	Pd	46	106.4	2.2
Phosphorus	P	15	30.9738	2.1
Platinum	Pt	78	195.09	2.2
Plutonium	Pu	94	(244)	1.3
Polonium	Po	84	(210)	2.0
Potassium	K	19	39.098	0.8
Praseodymium	Pr	59	140.908	1.1
Promethium	Pm	61	(147)	1.1
Protactinium	Pa	91	231.036	1.4
Radium	Ra	88	226.025	0.9
Radon	Rn	86	(222)	
Rhenium	Re	75	186.207	1.9
Rhodium	Rh	45	102.906	2.2
Rubidium	Rb	37	85.4678	0.8
Ruthenium	Ru	44	101.07	2.2
Rutherfordium	Rf	104	(261)	
Samarium	Sm	62	150.4	1.1
Scandium	Sc	21	44.9559	1.3
Selenium	Se	34	78.96	2.4
Silicon	Si	14	28.086	1.8
Silver	Ag	47	107.868	1.9
Sodium	Na	11	22.9898	0.9
Strontium	Sr	38	87.62	1.0
Sulfur	S	16	32.06	2.5
Tantalum	Ta	73	180.948	1.5
Technetium	Tc	43	98.9062	1.9
Tellurium	Te	52	127.60	2.1
Terbium	Tb	65	158.925	1.1
Thallium	Tl	81	204.37	1.8
Thorium	Th	90	232.038	1.2
Thulium	Tm	69	168.934	1.1
Tin	Sn	50	118.69	1.8
Titanium	Ti	22	47.90	1.5
Tungsten	W	74	183.85	1.7
Uranium	U	92	238.029	1.5
Vanadium	V	23	50.9414	1.6
Xenon	Xe	54	131.30	
Ytterbium	Yb	70	173.04	1.1
Yttrium	Y	39	88.9059	1.2
Zinc	Zn	30	65.38	1.6
Zirconium	Zr	40	91.22	1.4

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Table 2. Constants and Conversion Factors
Constants

Constants

Avogadro constant, N_A	6.022×10^{23} mol^{-1}
Faraday constant, F	96,485 C mol^{-1}
Faraday constant, F	96.5 kJ mol^{-1}
Proton charge, e	1.602×10^{-19} C
Proton charge, e	4.80×10^{-19} esu
Electron mass, me	9.11×10^{-28} g
Planck constant, h	6.626×10^{-34} J s
Speed of light, c	2.998×10^{8} m/s
Gas constant, R	8.314 J/mol K
Boltzmann constant, k	1.381×10^{-23} J/K
Pi	3.14159

Conversion Factors

Natural logarithm base, e = 2.718
kJ = 4.184 x kcal
kcal = 23.1 x eV
kcal = 2.39×10^{-11} x erg
1 esu^2/cm = 1 erg
ln y = 2.303 x log y
1 eV = 96.49 kJ/mol
1 cm^{-1} = 0.01196 kJ/mol
1 atm = 101,325 Pa = 760 torr
1 Å (angstrom) = 10^{-10} m = 100 pm
1 amu = 1.66×10^{-24} g

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Table 3. Standard Enthalpies of Formation of Gaseous Atoms

Atom	ΔH_f^o(g) kJ/mol	Atom	ΔH_f^o(g) kJ/mol	Atom	ΔH_f^o(g) kJ/mol
Actinium	385	Holmium	301	Radium	159
Aluminum	326	Hydrogen	218	Radon	0
Antimony	262	Indium	243	Rhenium	770
Argon	0	Iodine	107	Rhodium	556
Arsenic	302	Iridium	665	Rubidium	86
Astatine	92	Iron	418	Ruthenium	643
Barium	180	Krypton	0	Samarium	205
Beryllium	324	Lanthanum	423	Scandium	378
Bismuth	207	Lead	196	Selenium	227
Boron	573	Lithium	161	Silicon	452
Bromine	112	Lutecium	426	Silver	284
Cadmium	112	Magnesium	148	Sodium	109
Calcium	178	Manganese	281	Strontium	164
Carbon	717	Mercury	61	Sulfur	279
Cerium	422	Molybdenum	658	Tantalum	782
Cesium	79	Neodymium	322	Technetium	677
Chlorine	121	Neon	0	Tellurium	197
Chromium	397	Neptunium	439	Terbium	389
Cobalt	425	Nickel	430	Thallium	182
Copper	338	Niobium	726	Thorium	576
Dysprosium	297	Nitrogen	473	Thulium	230
Erbium	318	Osmium	791	Tin	302
Europium	176	Oxygen	249	Titanium	470
Fluorine	79	Palladium	378	Tungsten	849
Francium	92	Phosphorus	315	Uranium	490
Gadolinium	397	Platinum	565	Vanadium	514
Gallium	286	Polonium	144	Xenon	0
Germanium	377	Potassium	90	Ytterbium	150
Gold	366	Praseodymium	355	Ytterium	423
Hafnium	619	Protactinium	527	Zinc	131
Helium	0	Radium	159	Zirconium	609

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Table 4. Ionization Energies of Gaseous Atoms (kJ/mol)

Atomic #		1	2	3	4
1	H	1,312			
2	He	2,372	5,251		
3	Li	520.3	7,298	11,815	
4	Be	899.5	1,757	14,849	21,007
5	B	800.7	2,427	3,660	25,026
6	C	1,086	2,353	4,621	6,223
7	N	1,402	2,856	7,475	9,445
8	O	1,314	3,388	5,301	7,469
9	F	1,681	3,374	6,051	8,408
10	Ne	2,081	3,952	6,122	9,370
11	Na	495.9	4,563	6,913	9,544
12	Mg	737.8	1,451	7,733	10,541
13	Al	577.6	1,817	2,745	11,578
14	Si	786.5	1,577	3,232	4,356
15	P	1,012	1,903	2,912	4,957
16	S	999.6	2,251	3,361	4,564
17	Cl	1,251	2,297	3,822	5,158
18	Ar	1,521	2,666	3,931	5,771
19	K	418.9	3,051	4,412	5,877
20	Ca	589.8	1,145	4,912	6,474
21	Sc	631	1,235	2,389	7,089
22	Ti	658	1,310	2,653	4,175
23	V	650	1,414	2,828	4,507
24	Cr	652.9	1,592	2,987	4,740
25	Mn	717.4	1,509	3,249	4,940
26	Fe	759.4	1,561	2,958	5,290
27	Co	758	1,646	3,232	4,950
28	Ni	736.7	1,753	3,394	5,300
29	Cu	745.5	1,958	3,554	5,330
30	Zn	906.4	1,733	3,833	5,730

Atomic #		1	2	3	4
31	Ga	578.8	1,979	2,963	6,200
32	Ge	762.2	1,537	3,302	4,411
33	As	947	1,798	2,736	4,837
34	Se	941.0	2,045	2,974	4,144
35	Br	1,140	2,100	3,500	4,560
36	Kr	1,351	2,368	3,565	5,070
37	Rb	403.0	2,632	3,900	5,080
38	Sr	549.5	1,064	4,210	5,500
39	Y	616	1,181	1,980	5,960
40	Zr	660	1,267	2,218	3,313

Atomic #		1	2	3	4
41	Nb	664	1,382	2,416	3,700
42	Mo	685.0	1,558	2,621	4,480
43	Tc	702	1,472	2,850	
44	Ru	711	1,617	2,747	
45	Rh	720	1,745	2,997	
46	Pd	805	1,875	3,177	
47	Ag	731.0	2,074	3,361	
48	Cd	867.7	1,631	3,616	
49	In	558.3	1,821	2,705	5,200
50	Sn	708.6	1,412	2,943	3,930

Atomic #		1	2	3	4
51	Sb	833.8	1,595	2,440	4,260
52	Te	869.3	1,790	2,698	3,610
53	I	1,008	1,846	3,200	
54	Xe	1,170	2,047	3,100	
55	Cs	375.7	2,420		
56	Ba	502.9	965.3		
57	La	538.1	1,067	1,850	4,820
58	Ce	527.4	1,047	1,949	3,547
59	Pr	523.2	1,018	2,086	3,761
60	Nd	529.6	1,035	2,130	3,899

Atomic #		1	2	3	4
61	Pm	535.9	1,052	2,150	3,970
62	Sm	543.3	1,068	2,260	3,990
63	Eu	546.7	1,085	2,405	4,110
64	Gd	592.6	1,167	1,991	4,250
65	Tb	564.7	1,112	2,114	3,839
66	Dy	571.9	1,126	2,200	4,001
67	Ho	580.7	1,139	2,204	4,100
68	Er	588.7	1,151	2,194	4,115
69	Tm	596.7	1,163	2,544	4,119
70	Yb	603.4	1,176	2,415	4,220

Atomic #		1	2	3	4
71	Lu	523.6	1,340	2,022	4,360
72	Hf	680	1,440	2,250	3,215
73	Ta	761			
74	W	770			
75	Re	760			
76	Os	840			
77	Ir	880			
78	Pt	870	1,791		
79	Au	890.1	1,980		
80	Hg	1,007	1,810	3,300	

Atomic #		1	2	3	4
81	Tl	589.4	1,971	2,878	
82	Pb	715.6	1,450	3,082	4,083
83	Bi	703.3	1,610	2,466	4,370
84	Po	812			
85	At	890			
86	Rn	1,037			
87	Fr	384			
88	Ra	509.4	971.9		
89	Ac	499			
90	Th	587			

Atomic #		1
91	Pa	568
92	U	584
93	Np	597
94	Pu	585
95	Am	578
96	Cm	581
97	Bk	601
98	Cf	608
99	Es	619
100	Fm	627
101	Md	635
102	No	642

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Table 5. Electron Affinities (EA)[a]

Atom	EA (kJ/mol)	Atom	EA (kJ/mol)	Atom	EA (kJ/mol)	Atom	EA (kJ/mol)
H	73	O	141	P	72	Cu	118
Li	60	F	328	S	200	Br	325
B	8	Na	53	Cl	349	I	295
C	122	Al	44	K	48	Se	195
N	0	Si	134	Ti	20	Te	190

$O^-(g) + e^- \varnothing O^{2-}(g)$ -798$S^-(g) + e^- \varnothing S^{2-}(g)$ -640

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[a]Electron affinities are defined as heat liberated (e.g., ΔH for $H(g) + e^- \varnothing H^-(g)$ is -73 kJ/mol).

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Table 6. Common Bond Energies (*D*) and Bond Lengths (r)

Hydrogen

Bond	*D* (kJ/mol)	r (pm)
H-H	432	74
H-B	389	119
H-C	411	109
H-Si	318	148
H-Ge	288	153
H-Sn	251	170
H-N	386	101
H-P	322	144
H-As	247	152
H-O	459	96
H-S	363	134
H-Se	276	146
H-Te	238	170
H-F	565	92
H-Cl	428	127
H-Br	362	141
H-I	295	161

Group 15

Bond	*D* (kJ/mol)	r (pm)
N-N	167	145
N=N	418	125
N≡N	942	110
N-O	201	140
N=O	607	121
N-F	283	136
N-Cl	313	175
P-P	201	221
P-O	335	163
P=O	544	150
P=S	335	186
P-F	490	154
P-Cl	326	203
P-Br	264	
P-I	184	
As-As	146	243
As-O	301	178
As-F	484	171
As-Cl	322	216
As-Br	458	233
As-I	200	254
Sb-Sb	121	
Sb-F	440	
Sb-Cl ($SbCl_5$)	248	
Sb-Cl ($SbCl_3$)	315	232

Group 14

Bond	*D* (kJ/mol)	r (pm)
C-C	346	154
C=C	602	134
C≡C	835	120
C-Si	318	185
C-Ge	238	195
C-Sn	192	216
C-Pb	130	230
C-N	305	147
C=N	615	129
C≡N	887	116
C-P	264	184
C-O	358	143
C=O	799	120
C≡O	1072	113
C-B	356	
C-S	272	182
C=S	573	160
C-F	485	135
C-Cl	327	177
C-Br	285	194
C-I	213	214

Group 13

Bond	*D* (kJ/mol))	r (pm)
B-B	293	
B-O	536	
B-F	613	
B-Cl	456	175
B-Br	377	

Group 16

Bond	*D* (kJ/mol)	r (pm)
O-O	142	148
O=O	494	121
O-F	190	142
S=O	522	143
S-S (S_8)	226	205
S=S	425	149
S-F	284	156
S-Cl	255	207
Se-Se	172	
Se=Se	272	215

Group 17

Bond	*D* (kJ/mol)	r (pm)
F-F	155	142
Cl-Cl	240	199
Br-Br	190	228
I-I	148	267
At-At	116	
I-O	201	
I-F	273	191
I-Cl	208	232
I-Br	175	

Group 18

Bond	*D* (kJ/mol)	r (pm)
Kr-F (KrF_2)	50	190
Xe-O	84	175
Xe-F	130	195

Group 14

Bond	*D* (kJ/mol)	r (pm)
Si-Si	222	233
Si-N	355	
Si-O	452	163
Si-S	293	200
Si-F	565	160
Si-Cl	381	202
Si-Br	310	215
Si-I	234	243
Ge-Ge	188	241
Ge-N	257	
Ge-F	470	168
Ge-Cl	349	210
Ge-Br	276	230
Ge-I	212	
Sn-F	414	
Sn-Cl	323	233
Sn-Br	273	250
Sn-I	205	270
Pb-F	331	
Pb-Cl	243	242
Pb-Br	201	
Pb-I	142	279

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Table 7. Standard Heats and Free Energies of Formation, and Absolute Entropies of Inorganic and Organic Substances

A. Elements and Inorganic Compounds

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (J/mol K)
$H_2(g)$	0	0	130.5
H(g)	218	203.3	114.6
Li(s)	0	0	28
Li(g)	155.2	122.2	138.5
$Li_2O(s)$	-595.8	-560.7	37.9
$Li_2O_2(s)$	-634.7	-564.8	56.5
LiH(s)	-90.4	-69.9	24.7
LiCl(s)	-408.8	-381.7	55.2
LiF(s)	-612.1	-584.1	36
LiI(s)	-271.1	-270.3	86.8
Na(s)	0	0	51
Na(g)	108.8	78.2	153.6
NaH(s)	-57.3	-33.5	40.0
NaF(s)	-569	-541	58.6
NaCl(s)	-410.9	-384.1	72.4
NaBr(s)	-359.8	-347.7	86.8
NaI(s)	-287.9	-286.1	98.5
$Na_2SO_4(s)$	-1384.5	-1266.9	149.4
$NaNO_2(s)$	-466.5	-365.7	116.3
$NaNO_3(s)$	-359.4	-284.6	103.8
$Na_2CO_3(s)$	-1130.9	-1047.7	136
$Na_2O(s)$	-415.9	-376.6	72.8
$Na_2O_2(s)$	-504.6	-430.1	95.0
$NaO_2(s)$	-260.7	-218.8	115.9
$NaC_2H_3O_2(s)$	-710.4	-607.3	123.0
NaOH(s)	-430.5	-377	52.3
K(s)	0	0	63.6
K(g)	90	61.1	160.2
KF(s)	-562.7	-533	66.5
KCl(s)	-436	-408.4	83
$KClO_3(s)$	-391.2	-290	143.1
$K_2O(s)$	-361.5	-318.8	94.1
$K_2O_2(s)$	-493.7	-418.4	102.1
$KO_2(s)$	-282.8	-248.5	116.7
KOH(s)	-425.9	-374.5	79
$KNO_2(s)$	-492.9	-393.3	133
$KClO_4(s)$	-433.5	-304.2	151
Rb(s)	0	0	69.5

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)
Rb(g)	85.8	56.5	169.9
RbF(s)	-549.4		75.3
RbCl(s)	-430.5	-407.8	95.9
$Rb_2O(s)$	-330.1	-292.9	
$Rb_2O_2(s)$	-425.5	-351.5	
$RbO_2(s)$	-263.6		
Cs(s)	0	0	82.8
Cs(g)	78.7	51	175.3
CsF(s)	-530.9	-525.5	92.8
CsCl(s)	-433	-414.5	101.2
CsI(s)	-336.8	-333.5	123.0
$Cs_2O(s)$	-317.6	-326.4	146.8
$Cs_2O_2(s)$	-402.5	-359.8	
$CsO_2(s)$	-259.4		
Be(s)	0	0	9.6
Be(g)	320.5	282.8	136
$BeCl_2(s)$	-511.7	-449.5	75.8
Mg(s)	0	0	32.6
Mg(g)	150.2	115.5	148.5
$MgF_2(s)$	-1102.5	-1049.3	57.3
$MgCl_2(s)$	-641.8	-592.5	89.5
MgO(s)	-601.7	-559.4	26.8
$MgSO_4(s)$	-1278.2	-1173.6	91.6
$Mg(NO_3)_2(s)$	-789.5	-588.3	164
Ca(s)	0	0	41.6
Ca(g)	192.5	167.4	154.8
$CaH_2(s)$	-188.7	-149.8	41.8
CaO(s)	-635.5	-604.2	39.7
$Ca(OH)_2(s)$	-986.6	-896.6	76.1
$CaF_2(s)$	-1214.6	-1161.9	69
$CaCl_2(s)$	-795	-750.2	113.8
$CaCO_3(s)$	-1207.1	-1128.8	92.9
Sr(s)	0	0	54.4
Sr(g)	164	110	164.4
$SrCl_2(s)$	-828.4	-781.2	117.2
Ba(s)	0	0	66.9
Ba(g)	175.7	144.8	170.3
$BaCl_2(s)$	-860.2	-810.9	125.5

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)
$BaCl_2 \cdot 2H_2O(s)$	-1461.9	-1295.8	202.9
$BaCO_3(s)$	-1218.8	-1138.9	112.1
B(s)	0	0	6.7
$B_2O_3(s)$	-1263.6	-1184.1	54
BF(g)	-1136.8	-1120.5	254
$BCl_3(g)$	-402.9	-387.9	290
$B_2H_6(g)$	31.4	82.8	233
Al(s)	0	0	28.5
$Al_2O_3(s)$	-1669.8	-1576.5	51
$Al_2(SO_4)_3(s)$	-3440.9	-3506.6	239.3
C(s, graphite)	0	0	5.9
C(s, diamond)	2.1	2.9	2.5
C(g)	718.4	672.8	158.2
CF(g)	-933	-888.3	261.5
CCl(g)	-100.4	-58.2	310
$CCl_2(l)$	-132.6	-62.8	216.3
$C_3O(g)$	-220.9	-206.7	283.7
CO(g)	-110.5	-137.2	197.9
$CO_2(g)$	-393.3	-394.6	213.8
OCS(g)	-138.5	-165.7	231.4
$CS_2(g)$	117.2	66.9	237.7
HCN(g)	130.5	120.1	201.7
Si(s)	0	0	19
SiO(g)	-859.4	-856.7	41.8
SiH(g)	34.3	57.0	203.8
$SiCl_4(g)$	-609.6	-569.9	331.4
$SiCl_4(l)$	-640.2	-572.8	239.3
Ge(s)	0	0	42.2
$GeCl4(l)$	-543.9	-462.8	245.6
Sn(s)	0	0	51.5
SnO(s)	-286.2	-257.3	56.5
$SnO_2(s)$	-580.7	-520.5	52.3
$SnCl_2(s)$	-349.8		129.7
$SnCl_4(l)$	-545.2	-440.1	258.6
$N_2(g)$	0	0	191.6
NH(g)	45.6	-16.3	192.5
$N_2H_4(g)$	95	159	238.5
NO(g)	90.4	86.6	210.5
$NO_2(g)$	33.9	51.9	239.7
$N_2O(g)$	81.6	103.8	220.1
$N_2O_4(g)$	9.6	98.3	304.2
$NH_4Cl(s)$	-315.5	-203.8	94.6
$NH_4NO_3(s)$	-365.3	-184.0	151.1
$NH_4NO_3(s)$	-264		

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)
$HNO_3(l)$	-173.2	-79.9	155.6
P(g, white)	0	0	44.4
P(g, red)	-18.4	-13.8	29.3
P(g, black)	-43.1		
$P_4O_{10}(s)$	-3012.5	-2697.8	228.9
$PH_3(g)$	9.2	18.4	210
$PCl_3(g)$	-278.7	-258.6	311.7
$PCl_5(g)$	-371.1	-296.6	352.7
As(s)	0	0	35.1
AsH(g)	66.4	68.9	222.7
Sb(s)	0	0	45.6
$SbCl_3(s)$	-382	-323.8	184.1
$SbCl_5(l)$	-440.2	-350.2	301.2
$O_2(g)$	0	0	205
$O_3(g)$	142.3	163.6	237.7
$H_2O(g)$	-241.8	-228.4	188.7
$H_2O(l)$	-285.8	-237.2	69.9
$H_2O_2(l)$	-187.4	-120.4	109.6
$OCl_2(g)$	76.1	93.7	266.5
$S_8(s, rhombic)$	0	0	31.8
$H_2S(g)$	-20.1	-33.1	205.9
$SF_6(g)$	-1096.2	-991.6	290.8
$SO_2(g)$	-296.2	-300.4	248.5
$SO_3(g)$	-395.4	-370.3	256.1
$H_2SO_4(l)$	-811.3	-690.1	156.9
Se(s)	0	0	42.3
$H_2Se(g)$	85.8	71.1	221.3
$SeO_2(s)$	-236		
Te(s)	0	0	49.8
$H_2Te(g)$	154.4	138.5	243.2
$F_2(g)$	0	0	203.3
HF(g)	-268.6	-270.7	173.6
$Cl_2(g)$	0	0	223
HCl(g)	-92.5	-95.4	186.6
$Br_2(l)$	0	0	152.3
$Br_2(g)$	30.5	3.3	245.2
HBr(g)	-36.4	-53.1	198.3
BrF(g)	-46	-61.5	229.3
$BrF_3(g)$	-313.8	-288.7	292.5
$I_2(s)$	0	0	116.7
$I_2(g)$	62.3	19.2	260.7
HI(g)	25.9	1.3	206.3
$IF_7(g)$	-816.3	-746	329.3
ICl(g)	-88.3	-22.6	172

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)
Co(s)	0	0	30.1
CoO(s)	-312.5	-269.9	109.2
Cr(s)	0	0	23.8
$Cr_2O_3(s)$	-1139.7	-1058.1	81.2
$CrCl_2(s)$	-395.4	-356.1	115.5
$CrCl_3(s)$	-556.5	-486.2	123
Fe(s)	0	0	27.2
FeO(s)	-266.5	-244.3	54
$Fe_2O_3(s)$	-822.2	-741	90
Ni(s)	0	0	30.1
$NiCl_2 \cdot 6H_2O(s)$	-2103.3	-1713.3	344.3
Ti(s)	0	0	30.5
$TiCl_4(l)$	-802.1	-737.2	252.3
$TiO_2(s)$	-944.7	-889.1	50.2
Cu(s)	0	0	33.5
CuO(s)	-157.3	-129.7	42.7
$CuCl_2 \cdot 2H_2O(s)$	-821.3	-656.1	167.4
$CuSO_4(s)$	-769.9	-661.9	113.4
Zn(s)	0	0	41.4
ZnO(s)	-348.1	-318.4	43.5
$ZnCl_2(s)$	-415.5	-369.4	111.7
Cd(s)	0	0	51.9
CdS(s)	-161.9	-156.5	64.9
Hg(l)	0	0	77.4
$HgCl_2(s)$	-230.1	-185.8	144.3
$Hg_2Cl_2(s)$	-264.8	-210.9	195.8
HgO(s)	-90.4	-58.6	72
Ag(s)	0	0	42.7
AgF(s)	-204.6	-229.6	84.0
AgCl(s)	-127.2	-109.6	96.2
AgBr(s)	-100.4	-96.9	107.1
AgI(s)	-61.8	-66.2	115.5
$AgNO_3(s)$	-123	-32.2	141

Table 7. Standard Heats and Free Energies of Formation, and Absolute Entropies of Inorganic and Organic Substances
B. Organic Compounds

Compound	State	ΔH_f° (kJ/mol)	ΔG_f°(kJ/mol)	S° (J/mol K)	Class
Methane	g	-74.9	-50.6	186	alkane
Ethane	g	-84.5	-33.0	230	alkane
Propane	g	-104.0	-23.0	270	alkane
Butane	g	-127.2	-17.0	310	alkane
Pentane	g	-146.4	-8.4	349	alkane
Pentane	l	-173.2	-9.5	263	alkane
Hexane	g	-167.2	-0.3	388	alkane
Hexane	l	-198.8	-4.4	296	alkane
2-Methylpropane	g	-135.6	-21.0	295	alkane
2-Methylbutane	g	-154.4	-14.8	344	alkane
2-Methylbutane	l	-179.9	-15.2	260	alkane
2,2-Dimethylpropane	g	-166.0	-15.2	306	alkane
Cyclopropane	g	53.1	104.4	237	alkane
Cyclobutane	g	27.0	110.0	265	alkane
Cyclopentane	g	-77.4	38.6	293	alkane
Cyclopentane	l	-105.9	36.4	49	alkane
Cyclohexane	g	-123.0	31.8	298	alkane
Cyclohexane	l	-156.2	26.7	204	alkane
cis-1,2-Dimethylcyclohexane	l	-211.9	31.5	274	alkane
trans-1,2-Dimethylcyclohexane	l	-218.4	25.2	273	alkane

Compound	State	ΔH_f° (kJ/mol)	ΔG_f°(kJ/mol)	S° (kJ/mol)	Class
Propene	g	20.4	62.7	267	alkene
1,3-Butadiene	g	110.2	150.7	279	alkene
1-Butene	g	-0.1	71.3	306	alkene
Z-2-Butene	g	-7.0	65.9	301	alkene
E-2-Butene	g	-11.2	63.0	296	alkene
2-Methylpropene	g	-16.9	58.1	294	alkene
2-Methyl-1-butene	g	-36.3	65.6	340	alkene
2-Methyl-2-butene	g	-42.6	59.7	339	alkene
3-Methyl-1-butene	g	-29.0	74.8	333	alkene
Cyclohexene	l	-38.8	101.6	216	alkene
Cyclohexene	g	-5.4	106.9	311	alkene
1-Methylcyclopentene	g	-5.4	102.1	326	alkene
3-Methylcyclopentene	g	8.7	115.0	331	alkene
4-Methylcyclopentene	g	14.8	121.6	329	alkene
Ethene	g	52.3	68.1	219	alkene
Ethyne	g	226.7	209.0	201	alkyne
Propyne	g	185.4	194.6	248	alkyne
1-Butyne	g	165.2	202.1	291	alkyne
2-Butyne	g	146.3	185.4	283	alkyne
Benzene	g	82.8	129.7	268	aromatic
Benzene	l	49.0	124.3	172	aromatic
Styrene	l	103.8	202.5	238	aromatic
Toluene	g	50.0	122.0	320	aromatic
Toluene	l	12.0	113.8	221	aromatic
Ethylbenzene	l	-12.5	119.7	255	aromatic
m-Xylene	l	-25.4	107.7	252	aromatic
o-Xylene	l	-24.4	110.5	246	aromatic
p-Xylene	l	-24.4	110.0	248	aromatic
n-Propylbenzene	l	-38.4	124.7	288	aromatic
Isopropylbenzene (cumene)	l	-41.2	124.3	280	aromatic
Nitrobenzene	l	15.9	146.2	224	aromatic

Compound	State	ΔH_f° (kJ/mol)	ΔG_f°(kJ/mol)	S° (kJ/mol)	Class
1,2-Dibromoethane	g	-99.2	-13.1	409	alkyl halide
1,3-Dichloropropane	g	-161.5	-82.6	367	alkyl halide
1-Bromobutane	g	-107.3	-12.9	370	alkyl halide
1-Bromopropane	g	-87.9	-22.5	331	alkyl halide
1-Chloro-2-methylpropane	g	-159.4	-49.7	354	alkyl halide
1-Chlorobutane	g	-147.3	-58.8	358	alkyl halide
1-Chloropropane	g	-130.1	-50.7	319	alkyl halide
2,3-Dibromobutane	g	-102.1	-11.9	395	alkyl halide
2-Bromo-2-methylpropane	g	-133.9	-28.2	332	alkyl halide
2-Bromobutane	g	-120.1	-25.8	370	alkyl halide
2-Bromopropane	g	-97.1	-27.2	316	alkyl halide
2-Chloro-2-methylpropane	g	-183.3	-64.1	322	alkyl halide
2-Chlorobutane	g	-161.5	-53.5	360	alkyl halide
2-Chloropropane	g	-146.4	-62.5	304	alkyl halide
Benzyl bromide	g	83.7	141.3	380	alkyl halide
Bromomethane	g	-37.7	-28.2	246	alkyl halide
Chloroform	g	-101.3	-68.5	296	alkyl halide
Chloroform	l	-132.2	-73.8	202	alkyl halide
Chloromethane	g	-86.3	-62.9	234	alkyl halide
Dichloromethane	g	-95.4	-68.9	270	alkyl halide
Dichloromethane	l	-124.3	-70.4	179	alkyl halide
Diiodomethane	g	122.0	101.4	310	alkyl halide
Fluoromethane	g	-233.9	-210.0	223	alkyl halide
Iodomethane	g	14.0	15.6	254	alkyl halide
Iodomethane	l	-13.8	15.1	163	alkyl halide
Tetrachloromethane	g	-95.8	-53.6	310	alkyl halide
Tetrafluoroethene	g	-649.0	-623.7	300	alkyl halide
Tetrafluoromethane	g	-933.0	-888.3	262	alkyl halide
Tribromomethane (bromoform)	g	25.1	15.8	331	alkyl halide
Trifluoromethane	g	-693.0	-658.9	259	alkyl halide

Compound	State	ΔH_f° (kJ/mol)	ΔG_f°(kJ/mol)	S° (kJ/mol)	Class
Methanol	l	-238.6	-166.2	127	alcohol
Methanol	g	-201.2	-162.5	240	alcohol
Ethanol	l	-277.0	-174.1	161	alcohol
Ethanol	g	-234.8	-168.3	283	alcohol
1-Propanol	l	-304.6	-170.7	193	alcohol
1-Propanol	g	-257.5	-163.0	325	alcohol
2-Propanol	l	-318.0	-180.4	181	alcohol
2-Propanol	g	-272.6	-173.6	310	alcohol
1-Butanol	l	-325.8	-161.1	226	alcohol
1-Butanol	g	-274.4	-150.7	363	alcohol
2-Butanol	g	-292.3	-167.3	359	alcohol
2-Methyl-2-propanol	g	-325.8	-191.0	326	alcohol
2-Methyl-2-propanol	l	-359.3	-184.8	193	alcohol
2-Methyl-2-propanol	s	-365.9	-184.8	171	alcohol
1-Pentanol	l	-357.9	-161.3	255	alcohol
1-Pentanol	g	-302.4	-149.7	403	alcohol
2-Methyl-2-butanol	l	-379.5	-175.2	229	alcohol
2-Methyl-2-butanol	g	-329.1	-165.8	367	alcohol
Cyclohexanol	l	-348.2	-133.3	200	alcohol
Cyclohexanol	g	-294.6	-117.9	328	alcohol
Benzyl alcohol	l	-161.0	-27.5	217	alcohol

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Diethyl ether (ether)	g	-252.2	-122.3	343	ether
Diethyl ether (ether)	l	-279.5	-122.9	253	ether
Dimethyl ether	g	-184.1	-112.9	267	ether
Diphenyl ether	l	-14.6	144.2	291	ether
Ethyl vinyl ether	g	-140.2			ether
Ethylene oxide	g	-52.6	-13.1	242	ether
Ethylene oxide	l	-77.4	-11.4	154	ether
Methyl ethyl ether	g	-216.4	-117.7	311	ether
Methyl isopropyl ether	g	-252.0	-120.9	338	ether
Methyl phenyl ether (anisole)	l	-128.5			ether
Methyl propyl ether	g	-237.7	-109.9	349	ether
Propylene oxide	g	-92.8	-25.8	287	ether
Propylene oxide	l	-120.7	-26.7	196	ether
Tetrahydrofuran	l	-216.2			ether
Benzaldehyde	l	-89.1	9.4		aldehyde
Butanal	g	-205.0	-114.8	345	aldehyde
Butanal	l	-238.7	-119.2	247	aldehyde
Ethanal	g	-166.4	-133.3	264	aldehyde
Methanal	g	-115.9	-109.9	219	aldehyde
2-Methylbutanal	l	-250.2			aldehyde
Propanal	g	-192.0	-130.5	305	aldehyde

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Ethyl ethanoate	l	-479.0	-332.7	259	ester
Ethyl methanoate	l	-399.3			ester
Ethyl propionate	l	-477.8	-331.2		ester
Methyl benzoate	l	-340.6			ester
Methyl ethanoate	l	-409.6			ester
Methyl methanoate	g	-349.8	-297.2	301	ester

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
2-Butanone	g	-238.4	-146.1	338	ketone
2-Butanone	l	-273.3	-151.4	239	ketone
2-Pentanone	g	-258.7	-137.1	376	ketone
2-Pentanone	l	-300.0	-147.5	272	ketone
2-Propanone (acetone)	g	-248.1	-153.1	295	ketone
2-Propanone (acetone)	l	-248.1	-155.4	200	ketone
3-Pentanone	g	-258.7	-135.3	370	ketone
Acetophenone	l	-142.5	-17.0	249	ketone
Cyclohexanone	g	-230.1	-90.8	322	ketone

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Phenol	g	-96.4	-32.9	316	phenol
Phenol	s	-165.0	-50.4	144	phenol
2-Nitrophenol	s	-210.5			phenol
3-Nitrophenol	s	-194.1			phenol
4-Nitrophenol	s	-194.1			phenol
2-Methylphenol (o-cresol)	g	-128.5	-37.1	358	phenol
3-Methylphenol (m-cresol)	g	-132.3	-40.5	357	phenol
4-Methylphenol (p-cresol)	g	-125.4	-30.9	348	phenol
Hydroquinone	s	-366.1	-207.0	140	phenol

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Acetyl chloride	g	-243.9	-206.2	295	acid halide
Benzoyl chloride	l	-164.4			acid halide
Benzoyl bromide	l	-106.7			acid halide
Acetic anhydride	g	-575.7	-476.7	390	anhydride
Acetic anhydride	l	-624.0	-488.8	269	anhydride
Benzoic anhydride	s	-431.4			anhydride
Acetamide	s	-317.6			amide
Formamide	l	-186.2	-141.0	248	amide
Acetanilide	s	-210.5			amide
Benzamide	s	-202.8			amide
Benzanilide	s	-90.0			amide

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Methylamine	g	-23.0	32.3	243	amine
Ethylamine	g	-46.0	37.3	285	amine
Dimethylamine	g	-18.8	68.0	273	amine
n-Propylamine	g	-72.4	39.8	324	amine
Trimethylamine	g	-23.8	98.9	289	amine
n-Butylamine	g	-92.0	49.2	363	amine
Diethylamine	g	-72.4	72.1	352	amine
2-Aminobutane	g	-104.2	40.6	351	amine
2-Amino-2-methylpropane	g	-119.9	28.9	338	amine
Triethylamine	g	-99.6	110.3	405	amine
N,N-Dimethylaniline	l	84.1	231.2	366	amine
N,N-Dimethylaniline	l	34.3	214.2	256	amine
N-Ethylaniline	g	56.1	207.4	352	amine
N-Ethylaniline	l	3.1	188.7	239	amine
Aniline	g	86.9	166.7	319	amine
Aniline	l	31.1	149.1	191	amine
2-Nitroaniline	s	-12.6	178.2	176	amine
3-Nitroaniline	s	-17.2	174.0	176	amine
4-Nitroaniline	s	-41.5	151.0	176	amine

Compound	State	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (kJ/mol)	Class
Acetonitrile	g	87.9	105.6	243	nitrile
Acetonitrile	l	53.1	98.9	150	nitrile
Benzonitrile	g	218.8	260.9	321	nitrile
Propionitrile	g	50.6	96.1	287	nitrile
Propionitrile	l	14.6	89.2	189	nitrile
Methyl radical	g	144	194	194	radical
Ethyl radical	g	111	243	248	radical
1-Propyl radical	g	87.9	287		radical
2-Propyl radical	g	73.6	279		radical
2-Methyl-1-propyl radical	g	35	302		radical
2-Methyl-1-propyl radical	g	57.3	315		radical
Allyl radical	g	170	260		radical
Benzyl radical	g	188	315		radical
Phenyl radical	g	328	290		radical
Cyclohexyl radical	g	54	318		radical
Cyclohexen-3-yl radical	g	126	314		radical
1,3-Cyclohexadien-5-yl	g	209	289		radical
Vinyl radical	g	289	236		radical
Trifluoromethyl radical	g	-465	-267		radical
Trichloromethyl radical	g	77.4	296		radical
Perfluoroethyl radical	g	-891	-341		radical
Ethynyl radical	g	510	208		radical
Methylene (carbene)	g	360	194		radical
Dichlorocarbene	g	197	267		radical
Difluorocarbene	g	-187	-241		radical
Methoxyoxyl radical	g	15	230		radical
Ethoxyl radical	g	-17	273		radical
2-Methyl-2-propoxyl radical	g	-90.4	317		radical
Acyl radical	g	-23	270		radical

[HOME]

Table 8. Standard Heats of Formation for Gaseous Complex Ions, Calculated and (Experimental)

Group	ΔH_f^o (kJ/mol)	Group	ΔH_f^o (kJ/mol)	Group	ΔH_f^o (kJ/mol)	Group	ΔH_f^o (kJ/mol)
OH^-	-209 (-143)	HS^-	-120	BF_4^-	-1701	IO_3^-	-208
NH_2^-	63	CN^-	36 (60)	NCO^-	-263	ClO_4^-	-344
BH_4^-	-96	N_3^-	144	SeO_4^{2-}	-502	CO_3^{2-}	-321
HF_2^-	627	O_2^-	(-49)	ClO_3^-	-200	HCO_3^-	-738
SO_4^{2-}	-758	O_2^{2-}	553	NO_3^-	-320	BrO_3^-	-145
CrO_4^{2-}	-705	$CH_3CO_2^-$	-554	$AlCl_4^-$	-1196	SiF_6^{2-}	-1328
$SnCl_6^{2-}$	-1156	$PbCl_6^{2-}$	-940	$TiCl_6^{2-}$	-1330	$HfCl_6^{2-}$	-1640
$PtCl_6^{2-}$	-792	$TiBr_6^{2-}$	-1142	NH_4^+	630	WBr_6^{2-}	-705

[HOME]

Table 9. Lattice Energy
A. Madelung Constants (A) for Common Crystal Lattices[a]

Structure	Constant
Sodium chloride	1.75
Cesium chloride	1.76
Zinc blende	1.64
Wurtzite	1.64
Fluorite	5.04
Rutile	4.82[b]
Corundum	25.03[b]

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[a] The Madelung constant, A, is used in the equation E = AZ 2e 2/r, where r is the sum of the ionic radii, e is the charge on an electron, and Z is the highest common denominator of the absolute values of the integral charges on the ions (e.g., for $MgCl_2$, Z = 1; for CaO, Z = 2).[b] Depends on exact structure.

[HOME]

Table 9. Lattice Energy

B. Values of Born Exponent to be Used in Repulsive Function for Lattice Energy[c]

Ion Type	Example	n
He-He	LiH	5
Ne-Ne	NaF, MgO	7
Ar-Ar	KCl, CaS, CuCl	9
Kr-Kr	RbBr, AgBr	10
Xe-Xe	CsI	12

[c]For compounds of mixed ion types, use the average value (e.g., for NaCl, n = 8).

[HOME]

Table 9. Lattice Energy

C. Lattice Energies (*E*) for Common Compounds

Compound	*E* (kJ/mol)	Compound	*E* (kJ/mol)	Compound	*E* (kJ/mol)
LiH	906	NaH	811	KH	714
LiF	1009	NaF	904	KF	801
LiCl	829	NaCl	769	KCl	698
LiBr	789	NaBr	736	KBr	672
LiI	734	NaI	688	KI	632
CuCl	979	AgF	969	AuCl	1042
CuBr	976	AgCl	916	AuI	1050
CuI	958	AgBr	900	TlCl	748
MgF_2	2908	AgI	895	BaF_2	2368
$MgBr_2$	2406	CaF_2	2611	TiF_2	2749
VF_2	2812	CaI_2	492	ZnF_2	2971
FeF_2	2912	CaO	3464	ZnS	3619
CuF_2	3042	CaS	3093	CdS	3402
MnF_2	2770	CrF_2	2879	HgS	3573
CoF_2	2962	NiF_2	3046	Al_2O_3	15,326

[HOME]

Table 9. Lattice Energy

D. Kapustinskii Equation

$E = 108{,}000\ Z_c Z_a \nu / r$, where Z_c and Z_a are absolute integral values of charges on the cation and anion, ν is the number of ions in the simplest formula, and r is the sum of the ionic radii. When r is in pm, E will result in kJ/mol.

[HOME]

Table 10. Contributions to Entropies of Solids at 298 K
A. Cation Contributions

Cation	J/mol K
Ag	54
Al	33
As	48
Au	64
B	21
Ba	57
Be	18
Bi	65
C	22
Ca	39
Cd	54
Ce	58
Co	44
Cr	43
Cs	57
Cu	45
Fe	44
Ga	47
Ge	47
Hf	62
Hg	64
In	54
Ir	64
K	38
La	58
Li	15
Mg	32
Mn	43
Mo	51
N	24
Na	31
Nb	51
Ni	44
Os	63
Pb	65
Pd	53
Pt	64
Ra	66
Rb	50
Re	63
Rh	52
Ru	52
Sb	55
Sc	41
Si	34
Sn	55
Sr	50
Ta	62
Tc	52
Ti	41
Tl	64
U	67
V	42
W	63
Y	50
Zn	46
Zr	51

[HOME]

Table 10. Contributions to Entropies of Solids at 298K

B. Anion Contributions, J/mol K

	Charge on Positive Ion			
Anion	**+1**	**+2**	**+3**	**+4**
F-	23	20	17	21
Cl-	42	34	29	34
Br-	54	46	42	38
I-	61	57	52	54
O^{2-}	10	2	2	4
S^{2-}	34	21	5	10

	Charge on Positive Ion			
Anion	**+1**	**+2**	**+3**	**+4**
Se^{2-}	67	48	33	
Te^{2-}	69	51	38	
OH^-	21	19	13	
CN^-	30	25		
NO_2^-	74	63		
NO_3^-	91	74	63	59
CO_3^{2-}	64	48	33	

	Charge on Positive Ion			
Anion	**+1**	**+2**	**+3**	**+4**
HCO_3^-	73	54	42	
$C_2O_4^{2-}$	92	74	59	
ClO_3^-	104	84		
BrO_3^-	111	96	79	
IO_3^-	107	92		
MnO_4^-	133	117		
SO_3^{2-}	79	62	46	
SO_4^{2-}	92	72	57	50
CrO_4^{2-}	110	88		
PO_4^{3-}	100	71	50	

[HOME]

Table 11. Group Contributions to $\Delta H_f^o(g)$ and $S^o(g)$ at 298 K[a]
A. Hydrocarbon Groups

Group	ΔH_f ° (kJ/mol)	S ° (J/mol K)	Group	ΔH_f ° (kJ/mol)	S ° (J/mol K)
$C-(H)_3(C)$	-42.1	127.1	$C-(C_d)(C)_2(H)$	-6.2	-48.9
$C-(H)_2(C)_2$	-20.7	39.4	$C-(C_d)(C_B)(H)_2$	-17.9	42.6
$C-(H)(C)_3$	-7.9	-50.4	$C-(C_B)(C)_2(H)$	-4.1	-51.0
$C-(C)_4$	2.1	-146.7	$C-(C_B)(C)(H)_2$	-20.3	38.9
$C_d-(H)_2$	26.2	115.4	$C-(C_B)(C)_3$	11.8	-147.0
$C_d-(H)(C)$	35.9	33.3	$C_B-(H)$	13.8	48.2
$C_d-(C)_2$	43.2	-53.1	$C_B-(C)$	23.0	-32.1
$C_d-(C_d)(H)$	28.3	26.7	$C_B-(C_d)$	23.7	-32.6
$C_d-(C_d)(C)$	37.1	-61.0	$[C_B-(C_t)]$	23.8	-32.6
$[C_d-(C_B)(H)]$	28.3	26.8	$C_B-(C_B)$	20.7	-36.1
$C_d-(C_B)(C)$	36.1	-61.0	$C-(C_t)(C)_2(H)$	-7.2	-46.8
$[C_d-(C_t)(H)]$	28.3	26.8	$C-(C_t)(C)(H)_2$	-19.8	43.0
$C-(C_d)(C)(H)_2$	-19.9	41.0	$C_t-(C)$	115.2	26.5
$C-(C_d)_2(H)_2$	-17.9	42.6	$C_t-(H)$	112.6	103.2
$C-(C_d)(C)_3$	7.0	-145.1	$C_t-(C_d)$	122.1	26.9
C_a	143.0	25.1	$C_t-(C_B)$	122.1	26.9

[a] The subscripts "d" and "t" designate carbon atoms in carbon-carbon double and triple bonds; "a", an allenic carbon; "B", an aromatic carbon; "A", a nitrogen atom in a nitrogen-nitrogen double bond; and "I", a nitrogen atom in a nitrogen-carbon double bond. Bracketed values are estimated.

[HOME]

Table 11. Group Contributions to ΔH_f^o(g) and S^o(g) at 298 K[a]

B. Corrections for Steric Interactions and Rings

	ΔH_f^o (kJ/mol)	S^o (J/mol K)
Alkane, *gauche* correction	3.3	
Alkene, *gauche* correction	2.1	
cis correction	4.2	
ortho correction	2.4	-6.7
Cyclopropane	115.4	134.2
Cyclopropene	224.5	140.4
Cyclobutane	110.5	124.6
Cyclobutene	124.6	121.2
Cyclopentane	26.3	114.1
Cyclopentene	24.6	107.8
Cyclohexane	0.0	78.6
Cyclohexene	5.9	90.0
Cycloheptane	26.8	66.5
Cycloheptene	22.6	
Cyclooctane	41.4	69.0

[HOME]

Table 11. Group Contributions to ΔH_f^o(g) and S^o(g) at 298 K[a]

C. Oxygen-Containing Groups

Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)	Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)
CO-(CO)(C)	-122.1		$O\text{-}(C)_2$	-99.1	36.3
$CO\text{-}(O)(C_d)$	-140.0		O-(C)(H)	-158.3	121.5
$CO\text{-}(O)(C_B)$	-192.3		C_d (CO)(O)	26.3	
CO-(O)(C)	-139.6	61.8	$CO\text{-}(C_d)(H)$	-132.5	
[CO-(O)(H)]	-123.3	146.0	C_d -(CO)(C)	39.3	
$CO\text{-}(C_B)_2$	-163.4		$[C_d\text{-}(CO)(H)]$	32.2	
$CO\text{-}(C_B)(C)$	-157.2		$[C_d\text{-}(O)(C_d)]$	37.2	
$[CO\text{-}(C_B)(H)]$	-132.5		$[C_d\text{-}(O)(C)]$	43.0	
$CO\text{-}(C)_2$	-131.7	62.7	$[C_d\text{-}(O)(H)]$	36.0	
CO-(C)(H)	-123.7	146.0	C_B -(CO)	40.5	

Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)	Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)
CO-(C)(H)	-123.7	146.0	C_B -(CO)	40.5	
$CO\text{-}(H)_2$	-115.8	224.3	C_B -(O)	-7.5	-42.6
$O\text{-}(CO)_2$	-212.8		$C\text{-}(CO)_2(H)_2$	-30.1	
O-(CO)(O)	-79.4		$C\text{-}(CO)(C)_3$	6.6	
$[O\text{-}(CO)(C_d)]$	-172.6		$C\text{-}(CO)(C)_2(H)$	-7.6	-50.2
O(CO)(C)	-172.6	35.1	$C\text{-}(CO)(C)(H)_2$	-20.9	40.1
O-(CO)(H)	-252.0	102.5	$[C\text{-}(CO)(H)_3]$	-42.1	127.1
O-(O)(O)	79.4	39.3	$C\text{-}(O)_2(C)_2$	-70.2	
O-(O)(C)	-18.8	39.3	$C\text{-}(O)_2(C)(H)$	-71.9	
O-(O)(H)	-68.0	116.4	$C\text{-}(O)_2(H)_2$	-74.0	

Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)	Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)
$O\text{-}(C_d)_2$	-137.1		$C\text{-}(O)(C_B)(H)_2$	-27.6	40.6
$O\text{-}(C_d)(C)$	-130.8		$C\text{-}(O)(C_d)(H)_2$	-28.8	
$O\text{-}(C_B)_2$	-80.7		$C\text{-}(O)(C)_3$	-27.6	-140.3
$O\text{-}(C_B)(C)$	-94.5		$C\text{-}(O)(C)_2(H)$	-29.3	-46.0
$[O\text{-}(C_B)(H)]$	-158.4	121.6	$C\text{-}(O)(C)(H)_2$	-35.5	43.0
$[C\text{-}(O)(H)_3]$	-42.1	127.1			

[a] The subscripts "d" and "t" designate carbon atoms in carbon-carbon double and triple bonds; "a", an allenic carbon; "B", an aromatic carbon; "A", a nitrogen atom in a nitrogen-nitrogen double bond; and "I", a nitrogen atom in a nitrogen-carbon double bond. Bracketed values are estimated.

[HOME]

Table 11. Group Contributions to ΔH_f^o(g) and S^o(g) at 298 K[a]

D. Nitrogen-Containing Groups

Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)	Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)
[C-(N)$(H)_3$]	-42.1	127.1	N_A-(N)	96.1	
C-(N)(C)$(H)_2$	-27.6	41.0	CO-(N)(H)	-123.7	146.0
C-(N)$(C)_2$(H)	-21.7	-48.9	CO-(N)(C)	-137.1	67.7
C-(N)$(C)_3$	-13.4	-142.5	N-$(CO)(H)_2$	-62.3	103.2
C-(N_A)(C)$(H)_2$	-23.0	41.0	N-(CO)(C)(H)	-18.4	16.3
C-$(N_A)(C)_2$(H)	-13.8	-48.9	N-$(CO)(C_B)$(H)	1.7	
C-$(N_A)(C)_3$	-7.9	-145.0	N-$(CO)_2$(H)	-77.3	
N-(C) $(H)_2$	20.1	124.2	N-$(CO)_2$(C)	24.7	
N-$(C)_2$(H)	64.4	37.4	N-$(CO)_2(C_B)$	-2.1	
N- $(C)_3$	102.0	-56.3	C-(CN)(C) $(H)_2$	94.0	168.0
N-(N) $(H)_2$	47.6	121.8	C-$(CN)(C)_2$(H)	107.8	82.8
N-(N)(C)(H)	87.4	40.2	C-(CN) $(C)_3$		-11.7
N-(N)(C)$_2$	122.1	-57.7	C-$(CN)_2(C)_2$		118.7
N-$(N)(C_B)$(H)	92.4		Cd-(CN)(H)	156.3	152.9
NI-(C)	89.0		Cd-(CN)$_2$	351.5	
NI-(C_B)	69.8		Ct-(CN)	266.7	148.0
C_B-(CN)	149.6	85.7	Cd-(NO_2)(H)		185.8
N_A-(H)	104.9	112.0	C-(NO_2)(C) $(H)_2$	-63.1	202.3
N_A-(C)	135.8	33.4	C-$(NO_2)(C)_2$(H)	-66.0	112.4
N-$(C_B)(H)_2$	20.1	124.2	C-$(NO_2)(C)_3$		16.3
N-(C_B)(C)(H)	62.3		C-$(NO_2)_2$(C)(H)	-62.3	
N-$(C_B)(C)_2$	109.5		O-(NO)(C)	-24.7	175.1
N-$(C_B)_2$(H)	68.1		O-$(NO)_2$(C)	-81.1	202.7
C_B-(N)	-2.1	-40.5			

[a] The subscripts "d" and "t" designate carbon atoms in carbon-carbon double and triple bonds; "a", an allenic carbon; "B", an aromatic carbon; "A", a nitrogen atom in a nitrogen-nitrogen double bond; and "I", a nitrogen atom in a nitrogen-carbon double bond. Bracketed values are estimated.

[HOME]

Table 11. Group Contributions to ΔH_f^o(g) and S^o(g) at 298 K[a]

E. Halogen-Containing Groups

Group	ΔH_f^o (kJ/mol)	S^o (J/mol K)
Cd-$(F)_2$	-324.3	156.1
Cd-$(Cl)_2$	-7.5	176.1
Cd-(F)(H)	-157.3	137.2
Cd-(Cl)(H)	8.8	148.1
Cd-(Br)(H)	53.1	160.2
Cd-(I)(H)	102.5	169.5
CB-(F)	-179.1	67.4
CB-(Cl)	-15.9	79.1
CB-(Br)	44.8	90.4
CB-(I)	100.4	99.2
C-(CB)$(F)_3$	-680.7	179.1
C-(CB)(Br)$(H)_2$	-28.9	0.0
C-(CB)(I)$(H)_2$	35.1	0.0
C-$(F)_3$(C)	-662.7	177.8
C-$(F)_2$(H)(C)	-457.3	163.6
C-(F)$(H)_2$(C)	-216.7	148.1
C-$(F)_2(C)_2$	-405.8	74.5
C-(F)(H)$(C)_2$	-202.5	58.6
C-(F)$(C)_3$	-183.7	0.0
C-$(F)_2$(Cl)(C)	-444.8	169.5
C-$(Cl)_3$(C)	-86.6	210.9
C-$(Cl)_2$(H)(C)	-79.1	182.8
C-(Cl)$(H)_2$(C)	-65.3	158.2
C-$(Cl)_2(C)_2$	-81.6	0.0
C-(Cl)(H)$(C)_2$	-53.6	73.6
C-(Cl)$(C)_3$	-53.6	-22.6
C-(Br)$(H)_2$(C)	-22.6	170.7
C-(Br)(H)$(C)_2$	-14.2	0.0
C-(Br)$(C)_3$	-1.7	-8.4
C-(I)$(H)_2$(C)	33.5	177.8
C-(I)(H)$(C)_2$	44.8	92.9
C-(I)$(C)_3$	54.4	0.0
C-(Cl)(C)(O)(H)	-93.3	64.4

[a] The subscripts "d" and "t" designate carbon atoms in carbon-carbon double and triple bonds; "a", an allenic carbon; "B", an aromatic carbon; "A", a nitrogen atom in a nitrogen-nitrogen double bond; and "I", a nitrogen atom in a nitrogen-carbon double bond. Bracketed values are estimated.

[HOME]

Table 12. Metallic, Covalent and Ionic Radii (r)[a]

(Note: 1 Å = 100pm)	
Atom/Ion	**r (pm)**
Ag	144
Ag^{+}	115
Al	143(140)
Al^{3+}	53
Ar	(95)
As	(122)
As^{3+}	58
Au	144
Au^{+}	137
B	(90)
Ba	224
Ba^{2+}	135
Be	112(125)
Be^{2+}	45
Bi	182
Bi^{3+}	103
Br	114
Br^{-}	196
C	(77)
Ca	197
Ca^{2+}	100
Cd	152
Cd^{2+}	95
Ce	182
Ce^{3+}	102
Cl	(99)
Cl-	184
Co	125
Co^{2+}	70
Co^{3+}	60
Cr	129
Cr^{3+}	62
Cs	272
Cs^{+}	167
Cu	128
Cu^{+}	77
Cu^{2+}	73
F	(71)
F^{-}	133
Fe	126
Fe^{2+}	70
Atom/Ion	**r (pm)**
Fe^{3+}	60
Ga	153
Ga^{3+}	62
Ge	139(122)
H	(37)
He	(32)
Hf	159
Hg	155
Hg^{2+}	102
I	(133)
I-	220
In	167
In^{3+}	80
Ir	136
Ir^{3+}	82
K	235
K^{+}	138
Kr	(110)
La	188
La^{3+}	103
Li	157
Li^{+}	76
Lu	172
Lu^{3+}	86
Mg	160
Mg^{2+}	72
Mn	137
Mn^{2+}	70
N	(75)
Na	191
Na^{+}	102
Ne	(69)
Ni	125
Ni^{2+}	70
O	(73)
O^{2-}	140
Os	135
P	(110)
Pb	175
Pb^{2+}	119
Pd	137
Atom/Ion	**r (pm)**
Pd^{2+}	86
Po	153
Pt	139
Pt^{2+}	80
Pt^{4+}	77
Rb	250
Rb^{+}	152
Rh	134
Rn	(145)
Ru	134
S	(102)
S^{2-}	184
Sb	161(143)
Sb^{3+}	76
Sc	164
Sc^{3+}	75
Se	(117)
Se^{2-}	198
Si	(118)
Sn	158(140)
Sn^{2+}	118
Sr	215
Sr^{2+}	118
Te	(135)
Te^{2-}	221
Th	180
Ti	147
Ti^{3+}	67
Tl	171
Tl^{+}	150
Tl^{3+}	88
U	156
V	135
V^{2+}	79
W	141
Xe	(130)
Y	182
Y^{3+}	90
Zn	137
Zn^{2+}	74
Zr	160

[a] Metallic radii for 12-coordination are given for all metals. Covalent radii are in parentheses. Ionic radii are for six-coordination.

Table 13. Thermochemical Radii
A. Anions

Ion	*r*(pm)	Ion	*r*(pm)	Ion	*r*(pm)	Ion	*r*(pm)
BO_3^{3-}	191	BF_4^-	232	$GeCl_6^{2-}$	328	WBr_6^{2-}	343
BrO_3-	154	BeF_4^{2-}	245	$IrCl_6^{2-}$	335	$ZnBr_4^{2-}$	299
CO_3^{2-}	178	CoF_6^{2-}	244	$PbCl_6^{2-}$	348	PtI_6^{2-}	342
ClO_3-	171	CrF_6^{2-}	252	$PdCl_6^{2-}$	319	SnI_6^{2-}	396
ClO_4^-	240	MnF_6^{2-}	256	$PtCl_4^{2-}$	293	ZnI_4^{2-}	323
CrO_4^{2-}	256	NiF_6^{2-}	249	$PtCl_6^{2-}$	313	BH_4^-	193
IO_3^-	122	SiF_6^{2-}	259	$RuCl_6^{2-}$	332	$CH_3CO_2^-$	162
IO_4^-	249	PtF_6^{2-}	296	$SeCl_6^{2-}$	326	CN^-	191
MnO_4^-	229	RhF_6^{2-}	264	$SnCl_6^{2-}$	349	CNS^-	213
NO_2^-	192	TiF_6^{2-}	289	$TiCl_6^{2-}$	331	N_3^-	195
NO_3^-	179	$AlCl_4^-$	295	UCl_6^{2-}	337	NCO^-	203
$PO4^{3-}$	238	BCl_4^-	310	WCl_6^{2-}	336	NH_2^-	130
$SeO_3$2-	239	HCl2-	201	$ZnCl_4^{2-}$	286	O_2^{2-}	173
SeO_4^{2-}	249	$CeCl_6^{2-}$	353	$PtBr_6^{2-}$	342	OH^-	133
SiO44-	240	$CoCl_4^{2-}$	319	$SnBr_6^{2-}$	363	OCN^-	159
SO_4^{2-}	258	$CuCl_4^{2-}$	321	$TeBr_6^{2-}$	359	HCO_2^-	158
TeO_4^{2-}	254	$FeCl_4^-$	358	$TiBr_6^{2-}$	352	HCO_3-	156
VO_3^-	182	$GaCl_4^-$	289	UBr_6^{2-}	319	HS^-	207

[HOME]

Table 13. Thermochemical Radii

B. Cations

Ion	*r*(pm)
$Cd(NH_3)_6^{2+}$	266
$Co(H_2O)_6^{2+}$	234
$Co(NH_3)_5Cl^{2+}$	236
$Co(NH_3)_6^{2+}$	260
$Fe(NH_3)_6^{2+}$	263
$Mg(H_2O)_6^{2+}$	235
$Mn(H_2O)_6^{2+}$	234
$Mn(NH_3)_6^{2+}$	265
NH_4^+	137
$N(CH_3)_4^+$	201
$Ni(H_2O)_6^{2+}$	229
$Ni(NH_3)_6^{2+}$	258
PH_4^+	157
$Zn(H_2O)_6^{2+}$	235
$Zn(NH_3)_6^{2+}$	264
Fr^+	172

[HOME]

Table 14. Standard Formation Data for Aqueous Ions

A. Cations

Ion	ΔH_f^o(kJ/mol)	ΔG_f^o(kJ/mol)	S^o(J/mol K)
H^+	0	0	0
Li^+	-278	-294	14
Na^+	-240	-262	59
K^+	-251	-282	103
Rb^+	-246	-282	124
Cs^+	-248	-282	133
Cu^+	72	50	41
Ag^+	106	77	73
Tl^+	5	-32	126
NH_4^+	-132	-79	113
Be^{2+}	-383	-380	-130
Mg^{2+}	-467	-455	-138
Ca^{2+}	-543	-554	-53
Sr^{2+}	-546	-559	-33
Ba^{2+}	-538	-561	10
Cr^{2+}	-144	-164	
Mn^{2+}	-221	-228	-74
Fe^{2+}	-89	-79	-138
Co^{2+}	-58	-54	-113
Ni^{2+}	-54	-46	-129
Cu^{2+}	65	66	-100
Zn^{2+}	-154	-147	-112
Cd^{2+}	-76	-78	-73
Hg^{2+}	171	164	-32
Sn^{2+}	-9	-27	-17
Pb^{2+}	-2	-24	10
Al^{3+}	-531	-485	-322
Ga^{3+}	-212	-159	-331
In^{3+}	-105	-98	-264
Tl^{3+}	197	215	-192
Cr^{3+}	-251	-205	
Fe^{3+}	-49	-5	-316
Co^{3+}	92	134	-305
$Ag(NH_3)_2^+$	-112	-18	242

[HOME]

Table 14. Standard Formation Data for Aqueous Ions

B. Anions

Ion	ΔH_f^o(kJ/mol)	ΔG_f^o(kJ/mol)	S^o(J/mol K)
F^-	-333	-279	-14
Cl^-	-167	-131	57
Br^-	-121	-104	83
I^-	-57	-52	107
ClO^-	-107	-37	42
ClO_2^-	-67	17	101
ClO_3^-	-99	-3	162
ClO_4^-	-129	-9	192
BrO_3^-	-84	2	163
IO_3^-	-221	-128	118
OH^-	-230	-157	-11
SH^-	-18	12	63
S_2^{2-}	33	86	-15
HSO_4^-	-887	-756	132
SO_3^{2-}	-635	-487	-29
SO_4^{2-}	-909	-745	20
SeO_3^{2-}	-509	-370	13
SeO_4^{2-}	-599	-441	54
NO_2^-	-105	-37	140
NO_3^-	-207	-111	146
N_3^-	275	348	108
PO_4^{3-}	-1290	-1032	-222
CO_3^{2-}	-677	-528	-57
HCO_3^-	-692	-587	91
CN^-	151	172	94
BF_4^-	-1575	-1487	180
MnO_4^-	-541	-447	191
CrO_4^{2-}	-881	-728	50
$Cr_2O_7^{2-}$	-1490	-1301	262

[HOME]

Table 15. Absolute Enthalpies of Hydration of Gaseous Ions

Ion	ΔH_h^o (kJ/mol)
H^+	-1091
Li^+	-520
Na^+	-406
K^+	-320
Rb^+	-296
Cs^+	-264
In^+	-344
Tl^+	-328
Cu^+	-593
Ag^+	-473
Au^+	-615
NH_4^+	-307
Be^{2+}	-2484
Mg^{2+}	-1926
Ca^{2+}	-1579
Sr^{2+}	-1446
Ba^{2+}	-1309
Ti^{2+}	1862
Cr^{2+}	-1908
Mn^{2+}	-1851
Fe^{2+}	-1950
Co^{2+}	-2010
Ni^{2+}	-2096
Cu^{2+}	-2099
Pt^{2+}	-2100
Zn^{2+}	-2047
Cd^{2+}	-1809
Hg^{2+}	-1829
Sn^{2+}	-1554
Pb^{2+}	-1485
Al^{3+}	-4680
Sc^{3+}	-3930
Y^{3+}	-4105
Ga^{3+}	-4701
In^{3+}	-4118
Tl^{3+}	-4108
Cr^{3+}	-4563
Fe^{3+}	-4429
Co^{3+}	-4653
F^-	-524
Cl^-	-378
Br^-	-348
I^-	-308
NO_3^-	-314
OH^-	-460

[HOME]

Table 16. Solubilities of Gases in Water at 293 K

Gas	Solubility[a]
Acetylene	0.117
Ammonia	52.9
Bromine	14.9
Carbon dioxide	0.169
Carbon monoxide	0.0028
Chlorine	0.729
Ethane	0.0062
Ethylene	0.0149
Hydrogen	0.00016
Hydrogen sulfide	0.385
Methane	0.0023
Nitrogen	0.0019
Oxygen	0.0043
Sulfur dioxide	11.28

[a]Grams of gas dissolved in 100 g of water when the total pressure above the solution is 1 atm.

[HOME]

Table 17. Solubilities of Inorganic Compounds in Water at 293 K (g per 100 g water)

Fluorides	
AlF_3	0.67
BaF_2	0.16
MnF_2	1.06
NiF_2	1.2
KF	94.9
AgF	172
NaF	4.06

Chlorides	
$AlCl_3$	45.8
NH_4Cl	37.2
$BaCl_2.2\ H_2O$	35.8
$CaCl_2.6\ H_2O$	74.5
CsCl	187
$CoCl_2$	52.9
$CuCl_2$	73.0
$FeCl_2$	62.5
$FeCl_3.6\ H_2O$	91.8
$PbCl_2$	1.00
LiCl	83.5
$MgCl_2$	54.6
$MnCl_2$	73.9
$HgCl_2$	98.0
$NiCl_2$	60.8
KCl	34.2
NaCl	35.9

Nitrates	
$Al(NO_3)_3$	73.9
NH_4NO_3	192
$Ba(NO_3)_2$	9.0
$Cd(NO_3)_2$	150
$Ca(NO_3)_2.4\ H_2O$	129
$CsNO_3$	23
$Co(NO_3)_2$	97.4
$Cu(NO_3)_2$	125
$Fe(NO_3)_2.6\ H_2O$	140
$Fe(NO_3)_3.9\ H_2O$	138
$Pb(NO_3)_2$	54.3
$LiNO_3$	70.1
KNO_3	31.6
$AgNO_3$	216
$NaNO_3$	87.6

Sulfates	
$Al_2(SO_4)_3$	36.4
$(NH_4)_2SO4$	75.4
$CdSO_4$	76.6
$CaSO_4.2\ H_2O$	0.26
$CoSO_4$	36.1
$CuSO_4.5\ H_2O$	32.0
$FeSO_4.7\ H_2O$	48
Li_2SO_4	34.8
$MgSO_4$	33.7
K_2SO_4	11.1
Ag_2SO_4	0.8
Na_2SO_4	19.5
$ZnSO_4$	53.8

Carbonates	
Li_2CO_3	1.33
K_2CO_3	111
Na_2CO_3	21.5

Perchlorates	
$Ba(ClO_4)_2.3\ H_2O$	336
$Cd(ClO_4)_2.6\ H_2O$	188
$Fe(ClO_4)_3$	368
$LiClO_4$	56.1
$KClO_4$	1.68
$NaClO_4$	201

[HOME]

Table 18. Solubility Product Constants, K_{sp}

Bromides	
$PbBr_2$	4.6×10^{-6}
Hg_2Br_2	1.3×10^{-22}
AgBr	7.7×10^{-13}

Carbonates	
$BaCO_3$	8.1×10^{-9}
$CdCO_3$	2.5×10^{-14}
$CaCO_3$	8.7×10^{-9}
$CuCO_3$	1.3×10^{-10}
$FeCO_3$	5×10^{-11}
$PbCO_3$	1.6×10^{-13}
$MgCO_3$	8×10^{-11}
$NiCO_3$	1.3×10^{-7}
Ag_2CO_3	1.3×10^{-11}
$SrCO_3$	1.3×10^{-9}
$ZnCO_3$	1.0×10^{-7}

Chlorides	
AgCl	1.8×10^{-10}
$PbCl_2$	1.0×10^{-4}
Hg_2Cl_2	2.0×10^{-18}

Cyanides	
$Hg_2(CN)_2$	5×10^{-40}
AgCN	1.6×10^{-14}

Chromates	
$PbCrO_4$	1.7×10^{-14}
Ag_2CrO_4	1.9×10^{-12}
$BaCrO_4$	2.3×10^{-10}
$CuCrO_4$	3.6×10^{-6}
$CaCrO_4$	7.1×10^{-4}
Hg_2CrO_4	2.0×10^{-9}

Fluorides	
BaF_2	1.6×10^{-6}
CaF_2	4×10^{-11}
LiF	5×10^{-3}
PbF_2	4×10^{-8}
MgF_2	6×10^{-9}
SrF_2	3×10^{-9}

Hydroxides	
$Al(OH)_3$	4×10^{-15}
$Cd(OH)_2$	2×10^{-14}
$Ca(OH)_2$	6×10^{-6}
$Cr(OH)_3$	7×10^{-31}
$Co(OH)_3$	1×10^{-43}
$Co(OH)_2$	3×10^{-16}
$Cu(OH)_2$	2×10^{-19}
$Fe(OH)_3$	6×10^{-38}
$Fe(OH)_2$	2×10^{-15}
$Pb(OH)_2$	4×10^{-15}
$Mg(OH)_2$	1.8×10^{-11}
$Mn(OH)_2$	2×10^{-13}
$Ni(OH)_2$	2×10^{-16}
$Zn(OH)_2$	5×10^{-17}

Iodides	
Hg_2I_2	5×10^{-29}
AgI	8×10^{-17}
PbI_2	1.4×10^{-8}

Oxalates	
BaC_2O_4	1.6×10^{-7}
CaC_2O_4	1.9×10^{-9}
MgC_2O_4	9.6×10^{-5}
SrC_2O_4	6.0×10^{-8}
$Ag_2C_2O_4$	8.9×10^{-12}
PbC_2O_4	3×10^{-11}

Phosphates	
Ag_3PO_4	1.4×10^{-16}
$Ca_3(PO_4)_2$	1×10^{-25}
$Mg_3(PO_4)_2$	4×10^{-25}

Sulfates	
$BaSO_4$	1.0×10^{-10}
$CaSO_4$	2×10^{-5}
$PbSO_4$	1.6×10^{-8}
Hg_2SO_4	7×10^{-7}
Ag_2SO_4	6×10^{-5}
$SrSO_4$	3×10^{-7}

Sulfides	
CdS	1×10^{-28}
CoS	1×10^{-22}
CuS	1×10^{-36}
FeS	1×10^{-18}
PbS	1×10^{-28}
MnS	1×10^{-11}
HgS	1×10^{-54}
NiS	1×10^{-22}
Ag_2S	1×10^{-50}
SnS	1×10^{-25}
ZnS	1×10^{-23}

Table 19. Acid and Base Dissociation Constants in Water at 298 K
A. Acid Constants

Compound	Ka	Compound	Ka
HF	3.5×10^{-4}	o-FC_6H_4COOH	5.4×10^{-4}
HOCl	3.0×10^{-8}	m-FC_6H_4COOH	1.4×10^{-4}
$HClO_2$	1.0×10^{-2}	p-FC_6H_4COOH	7.2×10^{-5}
H_2S	5.7×10^{-8}, 1.2×10^{-15}	o-ClC_6H_4COOH	1.2×10^{-3}
H_2SO_3	1.3×10^{-2}, 5.6×10^{-8}	m-ClC_6H_4COOH	1.5×10^{-4}
H_2Se	2.0×10^{-4}, 1.0×10^{-11}	p-ClC_6H_4COOH	1.0×10^{-4}
H_2Te	2.5×10^{-3}, 5.0×10^{-11}	o-$NO_2C_6H_4COOH$	7.0×10^{-3}
HNO_2	4.6×10^{-4}	m-$NO_2C_6H_4COOH$	3.4×10^{-4}
HCN	4.9×10^{-10}	p-$NO_2C_6H_4COOH$	3.9×10^{-4}
H_2CO_3	4.2×10^{-7}, 4.8×10^{-11}	p-$CH_3C_6H_4COOH$	4.2×10^{-5}
$H_2C_2O_4$	5.9×10^{-2}, 6.4×10^{-5}	p-$CH_3O_2C_6H_4COOH$	3.4×10^{-5}
H_3PO_4	7.5×10^{-3}, 6.2×10^{-8},	p-$H_2NC_6H_4COOH$	1.2×10^{-5}
	2.2×10^{-13}	C_2H_5SH	2.5×10^{-11}

Compound	Ka	Compound	Ka
$HOOCCH_2COOH$	1.5×10^{-3}, 2.0×10^{-6}	$BrCH_2COOH$	1.4×10^{-3}
HCOOH	1.8×10^{-4}	ICH_2COOH	7.6×10^{-4}
CH_3COOH	1.8×10^{-5}	CH_3CH_2COOH	1.3×10^{-5}
FCH_2COOH	2.2×10^{-3}	C_6H_5COOH	6.5×10^{-5}
$F_2CHCOOH$	6.0×10^{-2}	o-$C_6H_4(COOH)_2$	1.3×10^{-3}, 3.9×10^{-6}
F_3CCOOH	6.0×10^{-1}	C_6H_5OH	1.3×10^{-10}
$ClCH_2COOH$	1.4×10^{-3}	o-$NO_2C_6H_4OH$	6.8×10^{-8}
$Cl_2CHCOOH$	3.3×10^{-2}	m-$NO_2C_6H_4OH$	5.3×10^{-9}
Cl_3CCOOH	2.0×10^{-1}	p-$NO_2C_6H_4OH$	7.0×10^{-8}

[HOME]

Table 19. Acid and Base Dissociation Constants in Water at 298 K

B. Base Constants

Compound	Kb	Compound	Kb
NH_3	1.8×10^{-5}	$C_6H_5NH_2$	3.8×10^{-10}
H_2NNH_2	1.0×10^{-6}	$C_6H_5N(CH_3)_2$	1.0×10^{-9}
H_2NOH	1.1×10^{-8}	o-$FC_6H_4NH_2$	1.6×10^{-11}
$(CH_3)_3N$	6.5×10^{-5}	m-$FC_6H_4NH_2$	2.5×10^{-11}
$(C_2H_5)_3N$	4.0×10^{-4}	p-$FC_6H_4NH_2$	4.5×10^{-10}
$(C_2H_5)_2NH$	1.3×10^{-3}	o-$NO_2C_6H_4NH_2$	2.0×10^{-14}
$C_2H_5NH_2$	5.6×10^{-4}	m-$NO_2C_6H_4NH_2$	2.5×10^{-12}
$C_6H_5CH_2NH_2$	2.0×10^{-5}	p-$CH_3C_6H_4NH_2$	1.0×10^{-9}
$(C_2H_5)_3P$	5.0×10^{-8}	p-$CH_3OC_6H_4NH_2$	2.2×10^{-9}
$(C_2H_5)_3As$	5.0×10^{-12}	pyridine	1.4×10^{-9}

[HOME]

Table 20. Overall Formation Constants of Coordination Compounds

Halo Complexes		Amine Complexes	
AlF_6^{3-}	1×10^{20}	$Co(NH_3)_6^{2+}$	5.0×10^{4}
$AgCl_2^{-}$	3×10^{5}	$Co(NH_3)_6^{3+}$	4.6×10^{33}
$AgCl_4^{3-}$	5×10^{6}	$Ni(NH_3)_6^{2+}$	2.0×10^{8}
$HgCl_4^{2-}$	5.0×10^{15}	$Cu(NH_3)_2^{+}$	7.2×10^{10}
$AgBr_4^{3-}$	8×10^{9}	$Cu(NH_3)_4^{2+}$	1.1×10^{13}
$CdBr_4^{2-}$	6.0×10^{3}	$Ag(NH_3)_2^{+}$	1.6×10^{7}
$HgBr_4^{2-}$	1.0×10^{21}	$Zn(NH_3)_4^{2+}$	2.8×10^{9}
$PbBr_4^{2-}$	1×10^{4}	$Cd(NH_3)_4^{2+}$	3.0×10^{7}
AgI_4^{3-}	1.0×10^{14}		
CdI_4^{2-}	2.5×10^{6}		
HgI_4^{2-}	1.9×10^{30}		
PbI_4^{2-}	1.6×10^{6}		

Cyano Complexes	
$Cu(CN)_4^{3-}$	2.0×10^{30}
$Ni(CN)_4^{2-}$	1.0×10^{22}
$Fe(CN)_6^{3-}$	1.0×10^{31}
$Fe(CN)_6^{4-}$	1.0×10^{24}
$Ag(CN)_2^{-}$	1.0×10^{20}
$Cd(CN)_4^{2-}$	5.9×10^{18}
$Hg(CN)_4^{2-}$	3.0×10^{41}
$Zn(CN)_4^{2-}$	1.0×10^{17}

Other Complexes	
AgI_4^{3-}	1.0×10^{14}
$Ag(C_2O_4)^{-}$	2.8×10^{2}
$Fe(C_2O_4)_3^{3-}$	4.0×10^{21}
$Al(C_2O_4)_3^{3-}$	2.0×10^{16}
HgS_2^{2-}	3.5×10^{54}
$Fe(NCS)^{2+}$	1.1×10^{3}
$Hg(NCS)_4^{2-}$	7.8×10^{21}
$Pb(C_2H_3O_2)_4^{2-}$	1.0×10^{3}
$Cu(en)_2^{2+}$	4.0×10^{19}
$Ni(en)_3^{2+}$	3.0×10^{18}
$Co(en)_3^{2+}$	8.7×10^{13}
$Co(en)_3^{3+}$	4.9×10^{48}
$Ca(EDTA)^{2-}$	1.0×10^{11}
$Mg(EDTA)^{2-}$	4.4×10^{8}

[HOME]

Table 21. Vapor Pressure of Water from 0 ºC to 100 ºC

T ºC	P(torr)	T ºC	P(torr)	T ºC	P(torr)	T ºC	P (torr)
0	4.6	26	25.2	51	97.2	76	301.4
1	4.9	27	26.7	52	102.1	77	314.1
2	5.3	28	28.4	53	107.2	78	327.3
3	5.7	29	30.0	54	112.5	79	341.0
4	6.1	30	31.8	55	118.0	80	355.1
5	6.5	31	33.7	56	123.8	81	369.7
6	7.0	32	35.7	57	129.8	82	384.9
7	7.5	33	37.7	58	136.1	83	400.6
8	8.1	34	39.9	59	142.6	84	416.8
9	8.6	35	42.2	60	149.4	85	433.6
10	9.2	36	44.6	61	156.4	86	450.9
11	9.8	37	47.1	62	163.8	87	468.7
12	10.5	38	49.7	63	171.4	88	487.1
13	11.2	39	52.4	64	179.3	89	506.1
14	12.0	40	55.3	65	187.5	90	525.8
15	12.8	41	58.3	66	196.1	91	546.1
16	13.6	42	61.5	67	205.0	92	567.0
17	14.5	43	64.8	68	214.2	93	588.6
18	15.5	44	68.3	69	223.7	94	611.0
19	16.5	45	71.9	70	233.7	95	634.0
20	17.5	46	75.7	71	243.9	96	658.0
21	18.7	47	79.6	72	254.6	97	682.0
22	19.8	48	83.7	73	265.7	98	707.3
23	21.1	49	88.0	74	277.2	99	733.2
24	22.4	50	92.5	75	289.1	100	760.0
25	23.8						

[HOME]

Table 22. Hammett Sigma Constants[a]

Group	σmeta	σpara	σI	σ_v	π	E_s	MR
H	0.00	0.00	0.00	0.00	0.00	0.00	1.03
CH_3	-0.07	-0.17	-0.04	0.52	0.56	-1.24	5.65
C_2H_5	-0.07	-0.15	-0.05	0.56	1.02	-1.31	10.30
n-C_3H_7	-0.07	-0.13	-0.03	0.68	1.55	-1.60	14.96
i-C_3H_7	-0.07	-0.15	-0.03	0.76	1.53	-1.71	14.96
n-C_4H_9	-0.08	-0.16	-0.04	0.68	2.13	-1.63	19.61
t-C_4H_9	-0.10	-0.20	-0.07	1.24	1.98	-2.78	19.62
H_2C=CH*	0.05	-0.02	0.09	2.11	0.82		10.99
C_6H_5*	0.06	-0.01	0.10	2.15	1.96	-3.82	25.36
CH_2Cl	0.11	0.12	0.15	0.60	0.17	-1.48	10.49
CF_3	0.43	0.54	0.42	0.91	0.88	-2.40	5.02
CN	0.56	0.66	0.53	0.40	-0.57	-0.51	6.33
CHO	0.35	0.42	0.25		-0.65		6.88
$COCH_3$	0.38	0.50	0.29	0.50	-0.55		11.18
CO_2H*	0.37	0.45	0.39	1.45	-0.32		6.93
$Si(CH_3)_3$	-0.04	-0.07	-0.13	1.40	2.59		24.96
F	0.34	0.06	0.52	0.27	0.14	-0.46	0.92
Cl	0.37	0.23	0.47	0.55	0.71	-0.97	6.03
Br	0.39	0.23	0.50	0.65	0.86	-1.16	8.88
I	0.35	0.18	0.39	0.78	1.12	-1.40	13.94
OH	0.12	-0.37	0.29	0.32	-0.67	-0.55	2.85
OCH_3	0.12	-0.27	0.27	0.36	-0.02	-0.55	7.87
OCH_2CH_3	0.10	-0.24	0.27	0.48	0.38		12.47
SH	0.25	0.15	0.26	0.60	0.39	-1.07	9.22
SCH_3	0.15	0.00	0.23	0.64	0.61	-1.07	13.82
NO_2*	0.71	0.78	0.76	1.39	-0.28	-2.52	7.36
NO	0.62	0.91	0.37		-0.12		5.20
NH_2	-0.16	-0.66	0.12		-1.23	-0.61	5.42
NHCHO	0.19	0.00	0.27		-0.98		10.31
$NHCOCH_3$	0.07	-0.15	0.26		-0.37		16.53
$N(CH_3)_2$	-0.15	-0.83	0.06	0.43	0.18		15.55
$N(CH_3)_3^+$	0.88	0.82	0.93	1.22	-5.96		21.20

[a] σ_{meta}, σ_{para} = Hammett constants; σ_I = inductive sigma constant; σ_v = Charton's v (size) values; π = hydrophobicity parameter; E_s = Taft size parameter; MR = molar refractivity (polarizability) parameter. An asterisk indicates that the group is in the most sterically hindered conformation.

[HOME]

Table 23. Standard Electrode Potentials

A. Acidic Media

Half-reaction		*E*º, V
$F_2(g) + 2H^+ + 2e^-$	$= 2HF(aq)$	3.06
$F_2 + 2e^-$	$= 2\ F^-$	2.87
$S_2O_8^{2-} + 2e^-$	$= 2SO_4^{2-}$	2.01
$Co^{3+} + e^-$	$= Co^{2+}$	1.82
$H_2O_2 + 2H^+ + 2e^-$	$= 2H_2O$	1.78
$MnO_4^- + 4H^+ + 3e^-$	$= MnO_2(s) + 2H_2O$	1.70
$H_5IO_6 + H^+ + 2e^-$	$= IO_3^- + 3H_2O$	1.64
$Ce^{4+} + e^-$	$= Ce^{3+}$	1.61
$BrO_3^- + 6H^+ + 5e^-$	$= 1/2\ Br_2(l) + 3H_2O$	1.52
$MnO_4^- + 8H^+ + 5e^-$	$= Mn^{2+} + 4H_2O$	1.51
$PbO_2 + 4H^+ + 2e^-$	$= Pb^{2+} + 2H_2O$	1.46
$Cl_2 + 2e^-$	$= 2Cl^-$	1.36
$Cr_2O_7^{2-} + 14H^+ + 6e^-$	$= 2Cr^{3+} + 7H_2O$	1.33
$MnO_2(s) + 4H^+ + 2e^-$	$= Mn^{2+} + 2H_2O$	1.23
$O_2(g) + 4H^+ + 4e^-$	$= 2H_2O(l)$	1.23
$IO_3^- + 6H^+ + 5e^-$	$= 1/2\ I_2 + 3H_2O$	1.20
$Br_2(aq) + 2e^-$	$= 2Br^-$	1.09
$VO_2^+ + 2H^+ + e^-$	$= VO^{2+} + H_2O$	1.00
$HNO_2 + H^+ + e^-$	$= NO(g) + H_2O$	1.00
$NO_3^- + 3H^+ + 2e^-$	$= HNO_2 + H_2O$	0.94
$2Hg^{2+} + 2e^-$	$= Hg_2^{2+}$	0.92
$Ag^+ + e^-$	$= Ag$	0.80
$Hg_2^{2+} + 2e^-$	$= 2Hg(l)$	0.79
$NO_3^- + 2H^+ + e^-$	$= NO_2 + H_2O$	0.78
$Fe^{3+} + e^-$	$= Fe^{2+}$	0.77
$O_2(g) + 2H^+ + 2e^-$	$= H_2O_2(aq)$	0.68
$Hg_2SO_4(s) + 2e^-$	$= 2Hg + SO_4^{2-}$	0.62
$H_3AsO_4(aq) + 2H^+ + 2e^-$	$= HAsO_2 + 2H_2O$	0.56
$I_3^- + 2e^-$	$= 3I^-$	0.54
$I_2 + 2e^-$	$= 2I^-$	0.54
$Cu^+ + e^-$	$= Cu$	0.52
$O_2 + 2H_2O + 4e^-$	$= 4OH^-$	0.40
$VO^{2+} + 2H^+ + e^-$	$= V^{3+} + H_2O$	0.36
$[Fe(CN)_6]^{3-} + e^-$	$= [Fe(CN)_6]^{4-}$	0.36
$Cu^{2+} + 2e^-$	$= Cu$	0.34
$UO_2^{2+} + 4H^+ + 2e^-$	$= U^{4+} + 2H_2O$	0.33
$BiO+ + 2H^+ + 3e^-$	$= Bi + H_2O$	0.32
$Hg_2Cl_2(s) + 2e^-$	$= 2Hg + 2Cl^-$	0.27
$AgCl(s) + e^-$	$= Ag + Cl^-$	0.22
$SbO^+ + 2H^+ + 3e^-$	$= Sb + H_2O$	0.21
$SO_4^{2-} + 4H^+ + 2e^-$	$= H_2SO_3 + H_2O$	0.17
$Sn^{4+} + 2e^-$	$= Sn^{2+}$	0.15
$S(rhombic) + 2H^+ + 2e^-$	$= H_2S(aq)$	0.14
$CuCl + e^-$	$= Cu + Cl^-$	0.14
$TiO^{2+} + 2H^+ + e^-$	$= Ti^{3+} + H_2O$	0.10
$S_4O_6^{2-} + 2e^-$	$= 2S_2O_3^{2-}$	0.09
$AgBr(s) + e^-$	$= Ag + Br^-$	0.07
$2H^+ + 2e^-$	$= H_2(g)$	0.00
$Pb^{2+} + 2e^-$	$= Pb$	-0.13
$Sn^{2+} + 2e^-$	$= Sn(white)$	-0.14
$AgI(s) + e^-$	$= Ag + I^-$	-0.15
$Mo^{3+} + 3e^-$	$= Mo$	-0.20
$Ni^{2+} + 2e^-$	$= Ni$	-0.25
$V^{3+} + e^-$	$= V^{2+}$	-0.26
$Co^{2+} + 2e^-$	$= Co$	-0.28
$[Ag(CN)_2]^- + e^-$	$= Ag + 2CN^-$	-0.31
$Cd^{2+} + 2e^-$	$= Cd$	-0.40
$Cr^{3+} + e^-$	$= Cr^{2+}$	-0.41
$Fe^{2+} + 2e^-$	$= Fe$	-0.44
$2CO_2 + 2H^+ + 2e^-$	$= H_2C_2O_4$	-0.49
$U^{4+} + e^-$	$= U^{3+}$	-0.61
$Cr^{3+} + 3e^-$	$= Cr$	-0.74
$Zn^{2+} + 2e^-$	$= Zn$	-0.76
$Mn^{2+} + 2e^-$	$= Mn$	-1.18
$Zr^{4+} + 4e^-$	$= Zr$	-1.53
$Ti^{2+} + 2e^-$	$= Ti$	-1.63
$Al^{3+} + 3e^-$	$= Al$	-1.66
$Th^{4+} + 4e^-$	$= Th$	-1.90
$Mg^{2+} + 2e^-$	$= Mg$	-2.37
$Ce^{3+} + 3e^-$	$= Ce$	-2.48
$La^{3+} + 3e^-$	$= La$	-2.52
$Na^+ + e^-$	$= Na$	-2.71
$Ca^{2+} + 2e^-$	$= Ca$	-2.87
$Sr^{2+} + 2e^-$	$= Sr$	-2.89
$Ba^{2+} + 2e^-$	$= Ba$	-2.91
$Cs^+ + e^-$	$= Cs$	-2.92
$K^+ + e^-$	$= K$	-2.92
$Li^+ + e^-$	$= Li$	-3.04

[HOME]

Table 23. Standard Electrode Potentials

B. Basic Media

Half-reaction		E^o, V
$ClO^- + H_2O + 2e^-$	$= Cl^- + 2OH^-$	0.89
$HO_2^- + H_2O + 2e^-$	$= 3OH^-$	0.88
$BrO^- + H_2O + 2e^-$	$= Br^- + 2OH^-$	0.76
$ClO_2^- + 2H_2O + 4e^-$	$= Cl^- + 4OH^-$	0.76
$ClO_3^- + 3H_2O + 6e^-$	$= Cl^- + 6OH^-$	0.62
$BrO_3^- + 3H_2O + 6e^-$	$= Br^- + 6OH^-$	0.61
$MnO_4^{2-} + 2H_2O + 2e^-$	$= MnO_2 + 4OH^-$	0.60
$MnO_4^- + 2H_2O + 3e^-$	$= MnO_2 + 4OH^-$	0.59
$IO^- + H_2O + 2e^-$	$= I^- + 2OH^-$	0.49
$O_2 + 2H_2O + 4e^-$	$= 4OH^-$	0.40
$ClO_4^- + H_2O + 2e^-$	$= ClO_3^- + 2OH^-$	0.36
$Ag_2O + H_2O + 2e^-$	$= 2Ag + 2OH^-$	0.34
$IO_3^- + 3H_2O + 6e^-$	$= I^- + 6OH^-$	0.26
$NO_3^- + H_2O + 2e^-$	$= NO_2^- + 2OH^-$	0.01
$O_2 + H_2O + 2e^-$	$= HO_2^- + OH^-$	-0.08
$2Cu(OH)_2 + 2e^-$	$= Cu_2O + 2OH^- + H_2O$	-0.09
$CrO_4^{2-} + 4H_2O + 3e^-$	$= Cr(OH)_3 + 5OH^-$	-0.12
$Cu(OH)_2 + 2e^-$	$= Cu + 2OH^-$	-0.22
$Bi_2O_3 + 3H_2O + 6e^-$	$= 2Bi + 6OH^-$	-0.46
$NO- + H_2O + e^-$	$= NO + 2OH^-$	-0.46
$S + H_2O + 2e^-$	$= HS^- + OH^-$	-0.48
$HPbO_2- + H_2O + 2e^-$	$= Pb + 3OH^-$	-0.54
$Fe(OH)_3 + e^-$	$= Fe(OH)_2 + OH^-$	-0.56
$PbO + H_2O + 2e^-$	$= Pb + 2OH^-$	-0.58
$Ni(OH)_2 + 2e^-$	$= Ni + 2OH^-$	-0.72
$Co(OH)_2 + 2e^-$	$= Co + 2OH^-$	-0.73
$Cd(OH)_2 + 2e^-$	$= Cd + 2OH^-$	-0.82
$2H_2O + 2e^-$	$= H_2 + 2OH^-$	-0.83

[HOME]

Table 24. Acid-Base Indicators

Indicator	pH Range	pKa	Colors[a]
Cresol red			R-Y
Thymol blue	1.2 to 2.8	1.65	R-Y
Methyl yellow	2.9 to 4.0	3.3	R-Y
Methyl orange	3.1 to 4.4	3.4	R-O
Bromophenol blue	3.0 to 4.6	3.85	Y-B
Bromocresol green	4.0 to 5.6	4.7	Y-B
Methyl red	4.4 to 6.2	4.95	R-Y
p-Nitrophenol	5.3 to 7.6	7.2	C-Y
Phenol red	6.4 to 8.0	7.9	Y-R
Thymol blue	8.0 to 9.6	8.9	Y-B
Phenolphthalein	8.0 to 10.0	9.4	C-R
Alizarin yellow R	10.0 to 12.0	11.2	Y-V

[a]B = blue, C = colorless, O = orange, R = red, V = violet, Y = yellow

[HOME]

Table 25. Oxidation-Reduction Indicators

Indicator	E^0, V	Color, Reduced-Oxidized Forms
Methylene blue	0.26	C-B
Diphenylamine	0.76	C-V
Sodium diphenylbenzidine sulfonate	0.87	C-V
Erioglaucine A	1.00	G-R
Tris(1,10-phenanthroline)iron(II) sulfate	1.06	R-B
Tris(5-nitro-1,10-phenanthroline)iron(II) sulfate	1.25	R-B

[HOME]

Table 26. Physical Characteristics of Solvents[a]

Solvent	mp	bp	D_4^{20}	n_D^{20}	ε	R_D	μ
Acetic acid	17	118	1.049	1.3716	6.15	12.9	1.68
Acetone	-95	56	0.788	1.3587	20.7	16.2	2.85
Acetonitrile	-44	82	0.782	1.3441	37.5	11.1	3.45
Anisole	-3	154	0.994	1.5170	4.33	33	1.38
Benzene	5	80	0.879	1.5011	2.27	26.2	0.00
Bromobenzene	-31	156	1.495	1.5580	5.17	33.7	1.55
Carbon disulfide	-112	46	1.274	1.6295	2.6	21.3	0.00
Carbon tetrachloride	-23	77	1.594	1.4601	2.24	25.8	0.00
Chlorobenzene	-46	132	1.106	1.5248	5.62	31.2	1.54
Chloroform	-64	61	1.489	1.4458	4.81	21	1.15
Cyclohexane	6	81	0.778	1.4262	2.02	27.7	0.00
Dibutyl ether	-98	142	0.769	1.3992	3.1	40.8	1.18
o -Dichlorobenzene	-17	181	1.306	1.5514	9.93	35.9	2.27
1,2-Dichloroethane	-36	84	1.253	1.4448	10.36	21	1.86
Dichloromethane	-95	40	1.326	1.4241	8.93	16	1.55
Diethylamine	-50	56	0.707	1.3864	3.6	24.3	0.92
Diethyl ether	-117	35	0.713	1.3524	4.33	22.1	1.30
1,2-Dimethoxyethane	-68	85	0.863	1.3796	7.2	24.1	1.71
N,*N* -Dimethylacetamide	-20	166	0.937	1.4384	37.8	24.2	3.72
N,*N* -Dimethylformamide	-60	152	0.945	1.4305	36.7	19.9	3.86
Dimethyl sulfoxide	19	189	1.096	1.4783	46.7	20.1	3.90
1,4-Dioxane	12	101	1.034	1.4224	2.25	21.6	0.45
Ethanol	-114	78	0.789	1.3614	24.5	12.8	1.69
Ethyl acetate	-84	77	0.901	1.3724	6.02	22.3	1.88
Ethyl benzoate	-35	213	1.050	1.5052	6.02	42.5	2.00
Formamide	3	211	1.133	1.4475	111.0	10.6	3.37
Hexamethylphosphoramide	7	235	1.027	1.4588	30.0	47.7	5.54
Isopropyl alcohol	-90	82	0.786	1.3772	17.9	17.5	1.66
Methanol	-98	65	0.791	1.3284	32.7	8.2	1.70
2-Methyl-2-propanol	26	82	0.786	1.3877	10.9	22.2	1.66
Nitrobenzene	6	211	1.204	1.5562	34.82	32.7	4.02
Nitromethane	-28	101	1.137	1.3817	35.87	12.5	3.54
Pyridine	-42	115	0.983	1.5102	12.4	24.1	2.37
Tetrahydrofuran	-109	66	0.888	1.4072	7.58	19.9	1.75
Toluene	-95	111	0.867	1.4969	2.38	31.1	0.43
Trichloroethylene	-86	87	1.465	1.4767	3.4	25.5	0.81
Triethylamine	-115	90	0.726	1.4010	2.42	33.1	0.87
Trifluoroacetic acid	-15	72	1.489	1.2850	8.55	13.7	2.26
2,2,2-Trifluoroethanol	-44	77	1.384	1.2910	8.55	12.4	2.52
Water	0	100	0.998	1.3330	80.1	3.7	1.82
o -Xylene	-25	144	0.880	1.5054	2.57	35.8	0.62

[a] Melting and boiling points in ûC, density (*D*) in g/mL at 20 ûC, refractive index (n_D) , dielectric constant (ε), molar refraction (R_D), and dipole moment (μ) in Debye at 20 ûC.

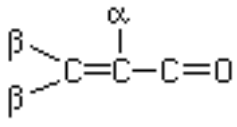
[HOME]

Table 27. Molal Freezing and Boiling Point Data

Solvent	K_f (°C kg/mol)	Mpt (°C)	K_b (°C kg/mol)	Bpt (°C)
Acetamide	4.04	80		221
Acetic acid	3.90	17	3.07	118
Acetone		-95	1.71	56
Aniline		-6	3.22	184
Antimony(III) chloride	17.95	73		220
Benzene	5.12	5	2.53	80
Bromobenzene		-31	6.26	156
Bromoform	14.4	8		150
2-Butanone		-87	2.28	80
DL-Camphor	37.7	177	5.611	204
Carbon disulfide		-112	2.35	46
Carbon tetrachloride	29.8	-23	5.03	77
Chlorobenzene		-46	4.15	132
Chloroform	4.68	-64	3.62	61
o -Cresol	5.60	31		191
p -Cresol	6.96	35		202
Cyclohexane	20.0	6	2.75	81
Cyclohexanol	39.3	25		161
Dibenzyl ether	6.27	4		298
1,2-Dibromoethane	12.5	9	6.608	131
Diethyl ether		-117	1.824	35
Dimethoxymethane		-105	2.125	42
N,*N* -Dimethylacetamide		-20	3.22	166
2,2-Dimethyl-1-propanol	11.0	53		113
Dimethyl sulfoxide	4.07	19		189
1,4-Dioxane	4.63	12	3.270	101
Diphenyl ether	7.88	27		258
Ethanol		-114	1.160	78
Ethyl acetate		-84	2.583	77
Formamide	3.85	3		211
Formic acid	2.77	8		101
Heptane		-91	3.43	98
N -Methylacetamide	6.65	31		206
Methyl acetate		-98	2.061	56
2-Methyl-2-propanol	8.37	26		82
Naphthalene	6.94	80	5.80	218
Nitrobenzene	6.852	6	5.24	211
Phenol	7.40	41	3.60	182
Piperidine		-10	2.84	106
1-Propanol		-126	1.59	97
Propionic acid		-21	3.51	140
Pyridine		-42	2.710	115
Sulfolane	64.1	27		285
1,1,2,2-Tetrabromoethane	21.7	0		244
Toluene		-95	3.29	111
Water	1.853	0	0.515	100
p -Xylene	4.3	13		138

[HOME]

Table 28. Additivity Rules for π-π* Transitions of Enones



Base values

Acylic ketones: 215 nm

6-membered cylic: 215 nm

5-membered cylic: 202 nm

Aldehydes: 210 nm

Carboxylic acids & esters : 195 nm

Increments

Alkyl groups,

a + 10 nm

b + 12 nm

g + 18 nm

Polar groups, -OH

a +35 nm

b +30 nm

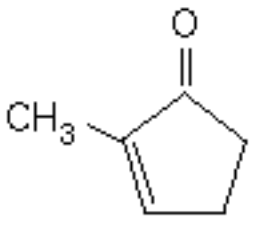
-Cl

a +15 nm

b +12 nm

Double bond extending conjugation +30 nm

For example:



202 (5-membered ring)
+10 (alkyl group, α)
+12 (ring residue, β)

224 nm

[HOME]

Table 29. Characteristic Infrared Absorptions

Group			Range, cm^{-1}	Intensity[a]
A. C-H	1.	Stretching vibrations		
		a. Alkanes	2962-2853	m-s
		b. Alkenes	3090-3010	m
		c. Alkynes	ca. 3300	s
		d. Aromatics	ca. 3030	v
		e. NCH_3, OCH_3	2850-2700	m
		f. CHO	2900-2820 and 2775-2700	w-m
	2.	Bending vibrations		
		a. CH	ca. 1340	w
		b. CH_2	1485-1445	m
		c. CH_3	1470-1430 and 1380-1370	s
		d. $C(CH_3)_2$	1385-1380 and 1370-1365	s
		e. $C(CH_3)_3$	1395-1385 and ca. 1365	s
		f. Aromatics		
		5 adj H	750 and 700	v, s
		4 adj H	750	v, s
		3 adj H	780	v, m
		2 adj H	830	v, m
		1 adj H	880	v, w
B. O-H	1.	Stretching vibrations		
		a. Free O-H	3650-3590	v, sh
		b. H-bonded	3550-3200	b
	2.	Bending vibrations		
		a. Alcohols	1430-1280	b, m
		b. Phenols	1390-1310	m
		c. Carboxylic acids	1440-1400	m
C. N-H	1.	Stretching vibrations		
		a. Primary amine, free	3500-3300 and 3420-3250	m-s
		b. Secondary amine	3500-3310	m
	2.	Bending vibrations	1650-1550	w-s
D. C=O	1.	Stretching vibrations		
		a. Ketones, aldehydes, carboxylic acids	ca. 1750-1660	s
		b. Acyl halides	1850-1750	s
		c. Amides	ca. 1710-1620	s
E. C=N		Stretching vibration	1690-1630	v
F. C≡N		Stretching vibration	2260-2220	m
G. C=C		Stretching vibration	1690-1560	w
H. C≡C		Stretching vibration	2275-2100	w-m
I. C_{ar}-C_{ar}		Skeletal vibrations in aromatics	ca. 1600 1580 1500 1450	w-m
J. C-O-C, C-O-H	1.	Stretching vibrations		
		a. Ethers: aliphatic, alkyl, aryl	ca. 1100 1280-1220 and 1050-1000	s
		b. Esters	1290-1180	b, s
	2.	Bending vibrations		
		a. Alcohols	1430-1280	m
		b. Phenols	1390-1310	m-s
K. C-X, X is a halogen		Stretching vibrations		
		a. Fluorides	1400-1000	s
		b. Chlorides	800-600	s
		c. Bromides	625-400	s
		d. Iodides	625-400	s

[a] v = variable; sh = sharp; b = broad; w = weak; m = medium; s = strong

[HOME]

Table 30. Properties of NMR-Active Nuclei
A. *I* = 1/2 Nuclei

Isotope	Natural Abundance (%)	Magnetogyric Ratio ($\gamma/10^7$, rad $T^{-1}s^{-1}$)	Relative Receptivity[a] (D^C)
^{1}H	99.985	26.7510	5.68×10^{3}
^{3}H		28.5335	
^{3}He	1.3×10^{-4}	-20.378	3.26×10^{-3}
^{13}C	1.108	6.7263	1.000
^{15}N	0.37	-2.7107	2.19×10^{-2}
^{19}F	100.0	25.1665	4.73×10^{3}
^{29}Si	4.70	-5.3141	2.09
^{31}P	100.0	10.829	3.77×10^{2}
^{57}Fe	2.19	0.8644	4.19×10^{-3}
^{77}Se	7.58	5.101	2.98
^{89}Y	100.0	-1.3106	0.668
^{103}Rh	100.0	-0.8420	0.177
^{107}Ag	51.82	-1.0828	0.197
^{109}Ag	48.18	-1.2449	0.276
^{111}Cd	12.75	-5.6720	6.97
^{113}Cd	12.26	-5.9330	7.59
^{115}Sn	0.35	-8.7475	0.705
^{117}Sn	7.61	-9.5301	19.8
^{119}Sn	8.58	-9.9707	25.2
^{123}Te	0.87	-7.011	0.903
^{125}Te	6.99	-8.453	12.5
^{129}Xe	26.44	-7.3995	31.8
^{169}Tm	100.0	-2.21	3.21
^{171}Yb	14.31	4.7117	4.44
^{183}W	14.40	1.1131	5.89×10^{-2}
^{187}Os	1.64	0.6161	1.14×10^{-3}
^{195}Pt	33.8	5.7505	19.1
^{199}Hg	16.84	4.7690	5.42
^{203}Tl	29.50	15.288	3.22×10^{2}
^{205}Tl	70.50	15.438	7.69×10^{2}
^{207}Pb	22.6	5.5968	11.8

[a]Relative to carbon-13.

[HOME]

Table 30. Properties of NMR-Active Nuclei
B. *I* > 1/2 Nuclei

Isotope	Spin	Natural Abundance (%)	Magnetogyric Ratio ($\gamma/10^7$, rad $T^{-1}s^{-1}$)	Quadrupole moment ($Q/10^{-28}$,m^2)	Relative Receptivity[a] (D^C)
^{2}H	1	0.015	4.1064	2.73×10^{-3}	8.21×10^{-3}
^{6}Li	1	7.42	3.9366	-8.0×10^{-4}	3.58
^{7}Li	3/2	92.58	10.396	-4.5×10^{-2}	1.54×10^{3}
^{9}Be	3/2	100.0	-3.7954	5.2×10^{-2}	78.8
^{10}B	3	19.58	2.8748	7.4×10^{-2}	22.1
^{11}B	3/2	80.42	8.5827	3.55×10^{-2}	7.54×10^{2}
^{14}N	1	99.63	1.9324	1.6×10^{-2}	5.69
^{17}O	5/2	0.037	-3.6266	-2.6×10^{-2}	6.11×10^{-2}
^{21}Ne	3/2	0.257	-2.1118		3.59×10^{-2}
^{23}Na	3/2	100.0	7.0760	0.12	5.25×10^{2}
^{25}Mg	5/2	10.13	-1.6370	0.22	1.54
^{27}Al	5/2	100.0	6.9706	0.149	1.17×10^{3}
^{33}S	3/2	0.76	2.0517	-6.4×10^{-2}	9.73×10^{-2}
^{35}Cl	3/2	75.53	2.6212	-7.89×10^{-2}	20.2
^{37}Cl	3/2	24.47	2.182	-6.21×10^{-2}	3.77
^{39}K	3/2	93.1	1.2484	5.5×10^{-2}	2.69
^{41}K	3/2	6.88	0.6852	6.7×10^{-2}	3.28×10^{-2}
^{43}Ca	7/2	0.145	-1.7999	0.2 ± 0.1	5.27×10^{-2}
^{45}Sc	7/2	100.0	6.4989	-0.22	1.71×10^{3}
^{47}Ti	5/2	7.28	-0.9313		0.864
^{49}Ti	7/2	5.51	-1.5083		1.18
^{51}V	7/2	99.76	7.032	0.3	2.16×10^{3}
^{53}Cr	3/2	9.55	-1.5120		0.490
^{55}Mn	5/2	100.0	6.598	0.55	9.94×10^{2}
^{59}Co	7/2	100.0	6.3171	0.40	1.57×10^{3}
^{63}Cu	3/2	69.09	7.0904	-0.16	3.65×10^{2}
^{65}Cu	3/2	30.91	7.5958	-0.15	2.01×10^{2}
^{67}Zn	5/2	4.11	1.6726	0.15	0.665
^{69}Ga	3/2	60.4	6.421	0.178	2.37×10^{2}
^{71}Ga	3/2	39.6	8.1578	0.112	3.19×10^{2}

Isotope	Spin	Natural Abundance (%)	Magnetogyric Ratio ($\gamma/10^7$, rad $T^{-1}s^{-1}$)	Quadrupole moment ($Q/10^{-28}$,m^2)	Relative Receptivity[a] (D^C)
^{73}Ge	9/2	7.76	-0.9332	-0.2	0.617
^{75}As	3/2	100.0	4.5816	0.3	1.43×10^{2}
^{79}Br	3/2	50.54	6.70	0.33	2.26×10^{2}
^{81}Br	3/2	49.46	7.2245	0.28	2.77×10^{2}
^{83}Kr	9/2	11.55	-1.029	0.15	1.23
^{85}Rb	5/2	72.15	2.5829	0.247	43.0
^{87}Rb	3/2	27.85	8.7532	0.12	2.77×10^{2}
^{87}Sr	9/2	7.02	-1.1594	0.36	1.07
^{93}Nb	9/2	100.0	6.5387	-0.2	2.74×10^{3}
^{95}Mo	5/2	15.72	1.743	0.12	2.88
^{97}Mo	5/2	9.46	-1.780	1.1	1.84
^{113}In	9/2	4.28	5.8496	1.14	83.8
^{115}In	9/2	95.72	5.8622	1.16	1.89×10^{3}
^{121}Sb	5/2	57.25	6.4016	-0.5	5.20×10^{2}
^{123}Sb	7/2	42.75	3.4668	-0.7	1.11×10^{2}
^{127}I	5/2	100.0	5.3521	-0.69	5.30×10^{2}
^{131}Xe	3/2	21.18	2.1935	-0.12	3.31
^{133}Cs	7/2	100.0	3.5089	-3.0×10^{-3}	2.69×10^{2}
^{135}Ba	3/2	6.59	2.6575	0.18	1.83
^{137}Ba	3/2	11.32	2.9729	0.28	4.41
^{139}La	7/2	99.911	3.7789	0.21	3.36×10^{2}
^{181}Ta	7/2	99.988	3.202	3.0	2.04×10^{2}
^{185}Re	5/2	37.07	6.0227	2.8	2.80×10^{2}
^{187}Re	5/2	62.93	6.0844	2.6	4.90×10^{2}
^{189}Os	3/2	16.1	2.0756	0.8	2.13
^{201}Hg	3/2	13.22	-1.7655	0.50	1.08
^{209}Bi	9/2	100.0	4.2988	-0.4	7.77×10^{2}

[HOME]

Table 31. Common NMR Solvents

Solvent	Mol. Wt.	D_4^{20} (g/mL)	mp[a]	bp[a]	δ_H (mult)[b]	δ_C (mult)[b]
Acetic acid-d_4	64.078	1.12	17	118	11.53 (1) 2.03 (5)	178.4 (br)
Acetone-d_6	64.117	0.87	-94	57	2.04 (5)	206.0 (13) 29.8 (7)
Acetonitrile-d_3	44.071	0.84	-45	82	1.93 (5)	118.2 (br) 1.3 (7)
Benzene-d_6	84.152	0.95	5	80	7.15 (br)	128.0 (3)
Carbon tetrachloride	153.81	1.59	-23	77		96.0 (1)
Chloroform-d	120.384	1.50	-64	62	7.24 (1)	77.0 (3)
Cyclohexane-d_{12}	96.236	0.89	6	81	1.38 (br)	26.4 (5)
Deuterium oxide	20.028	1.11	3.8	101.4	4.63[c] 4.67(Na_3PO4)	
Diglyme-d_{14}	148.263	0.95	-68	162	3.49 (br) 3.40 (br) 3.22 (br)	70.7 (5) 70.0 (5) 57.7 (7)
Dimethylformamide-d_7	80.138	1.04	-61	153	8.01 (br) 2.91 (5) 2.74 (5)	162.7 (3) 35.2 (7) 30.1 (7)
Dimethyl-sulfoxide-d_6	84.170	1.18	18	189	2.49 (5)	39.5 (7)
p-Dioxane-d_8	96.156	1.13	12	101	3.53 (m)	66.5 (5)
Methyl alcohol-d_4	36.067	0.89	-98	65	4.78 (1) 3.30 (5)	49.0 (7)
Methylene chloride-d_2	86.945	1.35	-95	40	5.32 (3)	53.8 (5)
Nitromethane-d_3	64.059	1.20	-29	101	4.33 (5)	62.8 (7)
Pyridine-d_5	84.133	1.05	-42	116	8.71 (br) 7.55 (br) 7.19 (br)	149.9 (3) 135.5 (3) 123.5 (3)
Tetrahydrofuran-d_8	80.157	0.99	-109	66	3.58 (br) 1.73 (br)	67.4 (5) 25.3 (br)
Toluene-d_8	100.191	0.94	-95	111	7.09 (m) 7.00 (br) 6.98 (m) 2.09 (m)	137.5 (l) 128.9 (3) 128.0 (3) 125.2 (3) 20.4 (7)
Trifluoroacetic acid-d	115.030	1.50	-15	72	11.50 (1)	164.2 (4) 116.6 (4)

[a] Melting and boiling points (ûC) are those of the corresponding light compound (except for D_2O).
[b] δ_H = chemical shift of residual protons; δ_C = ^{13}C chemical shift (both relative to TMS). Mult = multiplicity of peak (m = broad peak with fine structure; br = broad peak without fine structure).
[c] Since TMS is insoluble in water, reference is $(CH_3)_3Si(CH_2)_3SO_3Na$ (DSS).

[HOME]

Table 32. ^{13}C Chemical Shift Increments (ppm) for Substituted Alkanes

Substituent	α	β	γ
alkyl carbon (sp^3)	9.1	9.4	-2.5
-C=C- (sp^2)	19.5	6.9	-2.1
-C≡C- (sp)	4.4	5.6	-3.4
C_6H_5	22.1	9.3	-2.6
F	70.1	7.8	-6.8
Cl	31.0	10.0	-5.1
Br	18.9	11.0	-3.8
I	-7.2	10.9	-1.5
OH, OR	49.0	10.1	-6.2
-C(O)OR	56.5	6.5	-6.0
NH_2, NHR, NR_2	28.3	11.3	-5.1
NO_2	61.6	3.1	-4.6
CHO	29.9	-0.6	-2.7
C(O)R	22.5	3.0	-3.0
C(O)OH	20.1	2.0	-2.8
C(O)OR	22.6	2.0	-2.8
$CONR_2$	22.0	2.6	-3.2
CN	3.1	2.4	-3.3

[HOME]

Table 33. ^{13}C Chemical Shifts (ppm) of Carbonyl Derivatives XCOY

X	Y	δ
H	CH_3	199.7
H	$N(CH_3)_2$	162.4
CH_3	CH_3	205.8
CH_3	$CH=CH_2$	196.9
CH_3	C_6H_5	197.6
CH_3	OH	178.0
CH_3	OCH_3	170.6
CH_3	NH_2	172.7
CH_3	Cl	169.6
CH_3	Br	165.6
CH_3	I	158.9
C_6H_5	CH_3	196.9
C_6H_5	OH	184.8
C_6H_5	$N(CH_3)_2$	170.8
CF_3	OH	163.0
CF_3	OCH_2CH_3	158.1

[HOME]

Table 34. Additivity Parameters for ^{13}C Chemical Shifts in Substituted Benzenes[a]

Substituent	Ipso[b]	Ortho	Meta	Para
H	0.0	0.0	0.0	0.0
CH_3	8.9	0.7	-0.1	-2.9
C_2H_5	15.6	-0.4	0.0	-2.6
i -C_3H_7	20.2	-2.5	0.1	-2.4
t -C_4H_9	22.0	-3.4	-0.4	-3.1
$CH=CH_2$	9.5	-2.0	0.2	-0.5
C_6H_5	13.1	-1.1	0.4	-0.2
CF_3	2.6	-3.3	-0.3	3.2
OH	26.9	-12.7	1.4	-7.3
OCH_3	31.4	-14.4	1.0	-7.7
OC_2H_5	31.0	-13.7	1.1	-7.9
SCH_3	10.2	-1.8	0.4	-3.6
$C(O)H$	9.0	1.2	1.2	6.0
$C(O)OH$	2.1	1.5	0.0	5.1
$C(O)CH_3$	9.1	0.1	0.0	4.2
CN	-15.4	3.6	0.6	3.9
NH_2	18.0	-13.3	0.9	-9.8
$NHC(O)CH_3$	11.1	-9.9	0.2	-5.6
$N(CH_3)_2$	22.6	-15.6	1.0	-11.5
NO_2	20.0	-4.8	0.9	5.8
F	34.8	-12.9	1.4	-4.5
Cl	6.2	0.4	1.3	-1.9
Br	-5.5	3.4	1.7	-1.6
I	-32.0	10.2	2.9	1.0
$Si(CH_3)_3$	13.4	4.4	-1.1	-1.1
$Sn(CH_3)_3$	13.1	7.2	-0.4	-0.4

[a] Ppm relative to internal benzene. In CCl_4, except for $CH=CH_2$ (neat), $N(CH_3)_2$ (neat), $Si(CH_3)_3$ (neat), and $Sn(CH_3)_3$ (neat). Chemical shift of benzene: 128.5 ppm relative to TMS.

[b] Ipso refers to the carbon atom bearing the substituent.

[HOME]

Table 35. Proton, Carbon-13 and Nitrogen Chemical Shift Ranges

A. Proton[a]

Group	Range (ppm)
CH_3-C	0.5 - 1.5
CH_3-N	2.0 - 4.0
CH_3-O	3.0 - 4.0
CH_3-C=C	1.0 - 2.5
CH_3C=O	1.5 - 3.0
CH_3-C_6H_4R	2.0 - 3.0
CH_2-C	1.0 - 2.0
Cyclopropyl protons	-0.5 - 0.5
CH_2-X, X = halogen	2.0 - 4.5
CH_2-O	3.0 - 4.0
CH_2-N	2.0 - 4.0
CH_2-C=C	1.5 - 2.5
CH_2-C=O	2.0 - 3.0
CH_2-C_6H_4R	2.0 - 3.5
CH-C	0.5 - 1.5
CH-X, X = halogen	4.0 - 6.0
CH-O	3.5 - 5.5
CH-N	2.5 - 4.5
CH-C=O	2.0 - 3.0
CH-C_6H_4R	2.5 - 3.5
H-C≡C	2.0 - 3.0
Alkenes, nonconjugated	4.5 - 6.5
Alkenes, conjugated	5.5 - 7.5
H-C_6H_4R, aromatics	6.5 - 8.5
H-C_6H_4R, heteroaromatics	6.0 - 9.0
R-OH, alcohols	0.5 - 6.0
RNH_2	2.0 - 3.0
R_2NH	0.5 - 4.5
H-C=O, aldehydes	9.0 -10.5
RC(O)OH, acids	10.0 -13.0

[a] Relative to TMS.

[HOME]

Table 35. Proton, Carbon-13 and Nitrogen Chemical Shift Ranges

B. Carbon-13[a]

Group	Range (ppm)
CH_3-C	0 - 30
CH_3-N	10 - 50
CH_3-O	50 - 60
CH_2-C	20 - 45
Cyclopropyl carbons	0 - 10
CH_2-Br	25 - 45
CH_2-Cl	35 - 50
CH_2-N	35 - 55
CH_2-O	55 - 80
CH-C	30 - 55
CH-Br	45 - 60
CH-Cl	50 - 70
CH-N	50 - 75
CH-O	60 - 90
C-C	30 - 55
C-Br	60 - 75
C-Cl	70 - 85
C-N	55 - 75
C-O	70 - 90
C≡C	70 - 95
C≡N	110 - 130
C=C, benzenes; alkenes	105 - 150
C=C, heteroaromatics	105 - 150
C=N, heteroaromatics	145 - 150
C=O, anhydrides	150 - 175
C=O, esters	155 - 180
C=O, amides	160 - 180
C=O, acids	165 - 190
C=O, aldehydes	190 - 210
C=O, ketones	180 - 220

[a]Relative to TMS.

[HOME]

Table 35. Proton, Carbon-13 and Nitrogen Chemical Shift Ranges

C. Nitrogen[b]

Group or class	Range (ppm)
Amines, primary: RNH_2	-300 to -380
Amines, secondary: R_2NH	-280 to -360
Amines, tertiary: R_3N	-330 to -340
Ammonium ions	-270 to -360
Anilinium ions	-310 to -330
Aminophosphines	-280 to -330
Amides	-220 to -270
Isocyanates: RNCO	-320 to -350
Cyanates: ROCN	-190 to -210
Isothiocyanates: RNCS	-260 to -270
Thiocyanates: RSCN	-100 to -200
Nitriles: RCN	-120 to -140
Isonitriles: RNC	-180 to -220
Pyridines	-10 to -220
Imines: RCH=NH	-60 to -80
Nitro compounds: RNO_2	+40 to -30
Azo compounds: R-N=N-R	+180 to +130
Nitrosamines: R_2N-N=O	+190 to +130
Nitroso compounds: RN=O	+500 to +400

[b]Relative to NO_3^-. The ranges may be used to approximate both ^{14}N and ^{15}N chemical shifts.

[HOME]

Table 36. Character Tables For Common Symmetry Groups

A. The Nonaxial Groups

C_1	E
A	1

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_u	1	-1	x, y, z	

[HOME]

Table 36. Character Tables For Common Symmetry Groups

B. The C_n Groups

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	-1	x, y, R_x, R_y	yz, xz

C_3	E	C_3	C_3^2		$\varepsilon = \exp(2\pi i/3)$
A	1	1	1	z, R_z	x^2+y^2, z^2
E	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	ε	ε^*	$(x, y)(R_x, R_y)$	$(x^2-y^2, xy)(yz, xz)$
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	ε^*	ε		

C_4	E	C_4	C_2	C_4^3		
A	1	1	1	1	z, R_z	x^2+y^2, z^2
B	1	-1	1	-1		x^2-y^2, xy
E	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	i	-1	$-i$	$(x, y)(R_x, R_y)$	(yz, xz)
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	$-i$	-1	i		

C_5	E	C_5	C_5^2	C_5^3	C_5^4		$\varepsilon = \exp(2\pi i/5)$
A	1	1	1	1	1	z, R_z	x^2+y^2, z^2
E_1	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	ε	ε^2	ε^{2*}	ε^*	$(x, y)(R_x, R_y)$	(yz, xz)
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	ε^*	ε^{2*}	ε^2	ε		
E_2	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	ε^2	ε^*	ε	ε^{2*}		(x^2-y^2, xy)
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	ε^{2*}	ε	ε^*	ε^2		

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5		$\varepsilon = \exp(2\pi i/6)$
A	1	1	1	1	1	1	z, R_z	x^2+y^2, z^2
B	1	-1	1	-1	1	-1		
E_1	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	ε	$-\varepsilon^*$	-1	$-\varepsilon$	ε^*	(x, y) (R_x, R_y)	(xz, yz)
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	ε^*	$-\varepsilon$	-1	$-\varepsilon^*\varepsilon$			
E_2	$\begin{pmatrix} 1 & & \\ & 1 & \end{pmatrix}$	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		(x^2-y^2, xy)
	$\begin{pmatrix} & & \\ & & 1 \end{pmatrix}$	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$		

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Table 36. Character Tables For Common Symmetry Groups

C. The D_n Groups

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	-1	-1	z; R_z	xy
B_2	1	-1	1	-1	y; R_y	xz
B_3	1	-1	-1	1	x; R_x	yz

D_3	E	$2C_3$	$3C_2$		
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	-1	z; R_z	
E	2	-1	0	$(x,y)(R_x, R_y)$	$(x^2-y^2, xy)(xz, yz)$

D_4	E	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	-1	-1	z; R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x,y)(R_x, R_y)$	(xz, yz)

[HOME]

Table 36. Character Tables for Common Symmetry Groups
D. The C_{nv} Groups

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y)(R_x, R_y)$	$(x^2-y^2, xy)(xz, yz)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	-1	R_z	
E_1	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0		(x^2-y^2, xy)

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	-1	-1	2	0	0		(x^2-y^2, xy)

[HOME]

Table 36. Character Tables for Common Symmetry Groups

E. The C_{nh} Groups

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5		$\epsilon = \exp(2\pi i/3)$
A'	1	1	1	1	1	1	R_z	x^2+y^2, z^2
E'	1	ϵ	ϵ^*	1	ϵ	ϵ^*	(x, y)	(x^2-y^2, xy)
	1	ϵ^*	ϵ	1	ϵ^*	ϵ		
A''	1	1	1	-1	-1	-1	z	
E''	1	ϵ	ϵ^*	-1	$-\epsilon$	$-\epsilon^*$	(R_x, R_y)	(xz, yz)
	1	ϵ^*	ϵ	-1	$-\epsilon^*$	$-\epsilon$		

C_{4h}	E	C_4	C_2	C_4^3	i	S_4^3	σ_h	S_4		
A_g	1	1	1	1	1	1	1	1	R_z	x^2+y^2, z^2
B_g	1	-1	1	-1	1	-1	1	-1		x^2-y^2, xy
E_g	1	i	-1	$-i$	1	i	-1	$-i$	(R_x, R_y)	(xz, yz)
	1	$-i$	-1	i	1	$-i$	-1	i		
A_u	1	1	1	1	-1	-1	-1	-1	z	
B_u	1	-1	1	-1	-1	1	-1	1		
E_u	1	i	-1	$-i$	-1	$-i$	1	i	(x, y)	
	1	-1	-1	i	-1	i	1	$-i$		

[HOME]

Table 36. Character Tables for Common Symmetry Groups
F. The D_{nh} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		x^2+y^2, z^2
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x,y)	(x^2-y^2, xy)
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x,y)	

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
A_1'	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_2'	1	1	1	-1	1	1	1	-1	R_z	
E_1'	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	(x,y)	
E_2'	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0		(x^2-y^2, xy)
A_1''	1	1	1	1	-1	-1	-1	-1		
A_2''	1	1	1	-1	-1	-1	-1	1	z	
E_1''	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	-2	$-2\cos 72^\circ$	$-2\cos 144^\circ$ 0		(R_x, R_y)	(xz, yz)
E_2''	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0	-2	$-2\cos 144^\circ$	$-2\cos 72^\circ$	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0		(x^2-y^2, xy)
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1		
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0	(x,y)	
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0		

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Table 36. Character Tables For Common Symmetry Groups
G. The D_{nd} Groups

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1	z	xy
E	2	0	-2	0	0	(x,y); (R_x, R_y)	(xz, yz)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	-1	1	1	-1	R_z	
E_g	2	-1	0	2	-1	0	(R_x, R_y)	$(x^2-y^2, xy), (xz, yz)$
A_{1u}	1	1	1	-1	-1	-1		
A_{2u}	1	1	-1	-1	-1	1	z	
E_u	2	-1	0	-2	1	0	(x,y)	

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$		
A_1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	1	-1		
B_2	1	-1	1	-1	1	-1	1	z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	(x,y)	
E_2	2	0	-2	0	2	0	0		(x^2-y^2, xy)
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0	(R_x, R_y)	(xz, yz)

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Table 36. Character Tables For Common Symmetry Groups

H. The S_n Groups

S_4	E	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1	z	$x^2 - y^2, xy$
E	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}i\\-i\end{matrix}$	-1	$\begin{matrix}-i\\i\end{matrix}$	$(x, y); (R_x, R_y)$	(xz, yz)

S_6	E	C_3	C_3^2	i	S_6^5	S_6		$\epsilon = \exp(2\pi i/3)$
A_g	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_g	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	1	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	(R_x, R_y)	$(x^2 - y^2, xy); (xz, yz)$
A_u	1	1	1	-1	-1	-1	z	
E_u	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	-1	$\begin{matrix}-\epsilon\\-\epsilon^*\end{matrix}$	$\begin{matrix}-\epsilon^*\\-\epsilon\end{matrix}$	(x, y)	

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Table 36. Character Tables For Common Symmetry Groups
I. The Cubic Groups

T	E	$4C_3$	$4C_3^2$	$3C_2$		$\epsilon = \exp(2\pi i/3)$
A	1	1	1	1		$x^2 + y^2 + z^2$
E	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	$\begin{matrix}1\\1\end{matrix}$		$(2z^2 - x^2 - y^2,\ x^2 - y^2)$
T	3	0	0	-1	$(R_x, R_y, R_z);\ (x, y, z)$	$(xy;\ xz,\ yz)$

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2,\ x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	$(xy;\ xz,\ yz)$

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2 (= C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2 - x^2 - y^2,\ x^2 - y^2)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xz, yz, xy)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

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Table 36. Character Tables For Common Symmetry Groups
J. The Groups $C_{\infty v}$ and $D_{\infty h}$ for Linear Molecules

$C_{\infty v}$	E	$2C_{\infty}^{\Phi}$	...	$\infty\sigma_v$		
$A_1 \equiv \Sigma^+$	1	1	...	1	z	x^2+y^2, z^2
$A_2 \equiv \Sigma^-$	1	1	...	-1	R_z	
$E_1 \equiv \Pi$	2	$2\cos\Phi$	...	0	(x, y); (R_x, R_y)	(xz, yz)
$E_2 \equiv \Delta$	2	$2\cos 2\Phi$	...	0		(x^2-y^2, xy)
$E_3 \equiv \Phi$	2	$2\cos 3\Phi$	...	0		
...	...	...	...	...		

$D_{\infty h}$	E	$2C_{\infty}^{\Phi}$	...	$\infty\sigma_v$	i	$2S_{\infty}^{\Phi}$	...	∞C_2		
Σ_g^+	1	1	...	1	1	1	...	1		x^2+y^2, z^2
Σ_g^-	1	1	...	-1	1	1	...	-1	R_z	
Π_g	2	$2\cos\Phi$	...	0	2	$-2\cos\Phi$	...	0	(R_x, R_y)	(xz, yz)
Δ_g	2	$2\cos 2\Phi$	...	0	2	$2\cos 2\Phi$	...	0		(x^2-y^2, xy)
...	...	...	...	...	...	...	...	...		
Σ_u^+	1	1	...	1	-1	-1	...	-1	z	
Σ_u^-	1	1	...	-1	-1	-1	...	1		
Π_u	2	$2\cos\Phi$	...	0	-2	$2\cos\Phi$	...	0	(x, y)	
Δ_u	2	$2\cos 2\Phi$	...	0	-2	$-2\cos 2\Phi$	...	0		
...	...	...	...	...	...	...	...	...		

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Table 37. References

By Table:

1. J.E. Huheey, E.A.Keiter, and R.L. Keiter, "Inorganic Chemistry," 4th ed., Harper Collins, NY, 1993.

2. J.A. Dean, "Lange's Handbook of Chemistry," 14th ed., McGraw-Hill, NY, 1992, pps. 2-2 to 2-52.

3. W.E. Dasent, "Inorganic Energetics," 2nd ed., Cambridge University Press, NY, 1982, p. 35.

4. Dasent, pps. 44-47; C.E. Moore, "National Standard Reference Data Series," National Bureau of Standards, No. 34, Washington, DC, 1970; W.C. Martin, L. Hagan, J. Reader, and J. Sugar, J. Phys. Chem. Ref. Data, **3**, 771-9 (1974).

5. Dasent, pps. 57-58; H. Hotop and W.C. Lineberger, J. Phys. Chem. Ref. Data, **4**, 539-76 (1975).

6. Huheey, pps. A-21 to A-34; T.L. Cottrell, "The Strengths of Chemical Bonds," 2nd ed., Butterworths, London, 1958; B. deB. Darwent, "National Standard Reference Data Series," National Bureau of Standards, No. 31, Washington, DC, 1970; S.W. Benson, J. Chem. Educ., **42**, 502 (1965).

7. Lange's Handbook, pps. 6-1 to 6-147.

8. Hotop and Lineberger (experimental values); H.D.B. Jenkins and K.F. Pratt, Adv. Inorg. Chem. Radiochem., **22**, 1 (1979) (calculated values); R.C. Weast, Ed., "CRC Handbook of Chemistry and Physics," 62nd ed., CRC Press, Boca Raton, FL, 1981, pps. D-85 to D-86 (calculated values).

9. Huheey, pps. 99-134.

10. Dasent, p. 99; W.M. Latimer, "Oxidation Potentials," 2nd ed., Prentice-Hall, NY, 1952.

11. S.W. Benson, F.R. Cruickshank, D.M. Golden, G.R. Haugen, H.E. O'Neal, A.S. Rodgers, R. Shaw, and R. Walsh, Chem. Rev., **69**, 279 (1969).

12. A.F. Wells, "Structural Inorganic Chemistry," 5th ed., Clarendon Press, Oxford, 1984, p. 1288 (metallic radii for 12-coordination); Huheey, pp. 292 (covalent radii for nonmetals); R.D. Shannon, Acta Crystallogr., Sect. A: Found. Crystallogr., **32**, 751 (1976) (ionic radii for 6-coordination).

13. Dasent, p. 78; H.D.B. Jenkins and K.P. Thakur, J. Chem. Educ., **56**, 576 (1979).

14. Dasent, pps. 144-145.

15. Dasent, p. 152; D.W. Smith, J. Chem. Educ., **54**, 540 (1977).

16. G.W.C. Kaye and T.H. Laby, "Tables of Physical and Chemical Constants," 15th ed., Longman, NY, 1986, p. 219.

17. Kaye and Laby, pps. 184-196; Lange's Handbook, pps. 5-9 to 5-23.

18. Lange's Handbook, pps. 8-6 to 8-11; L.G. Sillen and A.E. Martell, "Stability Constants of Metal-Ion Complexes," The Chemical Society, London, 1964 (Special Publ. No. 17).

19. Lange's Handbook, pps. 8-13 to 8-71.

20. Lange's Handbook, pps. 8-83 to 8-103; Sillen and Martell.

21. Lange's Handbook, pps. 5-28 to 5-29.

22. C. Hansch and A. Leo, "Substituent Constants for Correlation Analysis in Chemistry and Biology," Wiley-Interscience, NY, 1979.

23. Huheey, pps. A-35 to A-37; A.J. de Bethune and N.A.S. Loud, "Standard Aqueous Electrode Potentials and Temperature Coefficients at 25 ûC," C.A. Hampel, Skokie, IL, 1964.

24. C.A. Streuli, in "Handbook of Analytical Chemistry," L. Meites, Ed., McGraw-Hill, NY, 1963, pps. 3-35 and 3-36.

25. I.M. Kolthoff and V.A. Stenger, "Volumetric Analysis," 2nd ed., Vol. 1, Interscience, NY, 1942, p. 140.

26. Lange's Handbook, pps. 5-91 to 5-125; A.J. Gordon and R.A. Ford, "The Chemist's Companion," Wiley-Interscience, NY, 1972, pps. 2-16.

27. Lange's Handbook, pps. 11-4 and 11-10 to 11-14.

28. R.M. Silverstein, G.C. Bassler, and T.C. Morrill, "Spectrometric Identification of Organic Compounds," 5th ed., Wiley, NY, 199l, pps. 302-303.

29. Silverstein, Bassler and Morrill, pps. 158-164.

30. R.K. Harris and B.E. Mann, Eds., "NMR and the Periodic Table," Academic Press, NY, 1978, pps. 5-7.

31. Merck, Sharpe & Dohme compilation.

32. D.W. Brown, J. Chem. Educ., **62**, 209 (1985); E. Pretsch, T. Clerc, J. Seibl, and W. Simon, "Tables of Spectral Data for Structure Determination of Organic Compounds," Springer-Verlag, NY, 1983, p. C90.

33. G.C. Levy, R.L. Lichter, and G.L. Nelson, "Carbon-13 Nuclear Magnetic Resonance Spectroscopy," 2nd ed., Wiley-Interscience, NY, 1980, pps. 136-156; E. Breitmaier and W. Voelter, "Carbon-13 NMR Spectroscopy," 3rd ed., VCH Publishers, Deerfield Beach, FL, 1987, pps. 215-232.

34. Levy, Lichter and Nelson, pps. 111-112; Breitmaier and Voelter, pps. 256-258.

35. Silverstein, Bassler and Morrill, Ch. 4 (proton data); Breitmaier and Voelter (carbon-13 data); G.C. Levy and R.L. Lichter, "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy," Wiley-Interscience, NY, 1979 (nitrogen data).

36. F.A. Cotton, "Chemical Applications of Group Theory," 3rd ed., Wiley-Interscience, NY, 1990.

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