

Contents

II/29 Molecular Constants

Subvolume A1

1	General Introduction.	1
1.1	General remarks	1
1.2	Review articles and tables	1
1.3	Arrangement of tables, substances and parameters	1
1.4	Error notation	2
1.5	Selection of data.	3
1.6	Abbreviations used for experimental methods	3
1.7	Selected fundamental constants and conversion factors	3
1.8	References for 1	5
2	Diamagnetic diatomic molecules: Introduction (W. HÜTTNER)	6
2.1	Defining equations for the parameters of diamagnetic diatomic molecules	6
2.1.1	Rovibrational and fine structure parameters	6
2.1.2	Hyperfine-interaction parameters	10
2.1.3	External-electric-field parameters	11
2.1.4	External-magnetic-field parameters	11
2.2	List of tabulated parameters of diamagnetic diatomic molecules	12
2.3	References	14
3	Data (W. HÜTTNER)	15
1	AgCl $X^1\Sigma^+$ Silver chloride.	15
2	AgF $X^1\Sigma^+$ Silver fluoride	16
3	AgH $X^1\Sigma^+$ Silver hydride	17
4	AgI $X^1\Sigma^+$ Silver iodide	19
5	AgO $X^2\Pi_i$ Silver oxide	20
6	AlAr $X^2\Pi_{1/2}$ Aluminum – argon (1/1)	21
7	AlBr $X^1\Sigma^+$ Aluminum bromide	22
8	AlCl $X^1\Sigma^+$ Aluminum chloride	23
9	AlF $X^1\Sigma^+$ Aluminum fluoride	24
10	AlH $X^1\Sigma^+$ Aluminum hydride	25
11	AlI $X^1\Sigma^+$ Aluminum iodide	27
12	AlNe $X^2\Pi_i$ Aluminum – neon (1/1)	28
13	AlO $X^2\Sigma^+$ Aluminum oxide	29
14	Al ₂ $X^3\Pi_u$ Dialuminum.	30
15	ArAu $X^2\Sigma$ Gold – argon (1/1)	31
16	ArB $X^2\Pi$ Boron – argon (1/1)	32
17	ArCa $X^1\Sigma^+$ Calcium – argon (1/1)	33
18	ArCa ⁺ $X^2\Sigma^+$ Calcium (1+) ion – argon (1/1)	35
19	ArCd $X0^+(^1\Sigma^+)$ Cadmium – argon (1/1)	36
20	ArCl $X1/2$ Argon chloride	38
21	ArCl ⁻ $X^1\Sigma^+$ Chloroargenate(1-)	39

22	ArGa	$X^2\Pi_{1/2}$	Gallium argon (1/1)	41
23	ArGe	$X^3\Sigma^-$	Germanium – argon (1/1)	42
24	ArH	$X^2\Sigma^+$, repulsive ground state	Argon hydride.	43
25	ArH ⁺	$X^1\Sigma^+$	Hydroargon (1+) ion	44
26	ArHe	$X^1\Sigma^+$ (0^+ in Hund's case c notation)	Argon – helium (1/1)	45
27	ArHe ⁺	$X^2\Sigma^+$	Argon (1+) ion – helium (1/1)	46
28	ArHg	$X0^+ (^1\Sigma^+)$	Mercury – argon (1/1)	47
29	ArIn	$X^2\Pi_{1/2}$	Indium – argon (1/1)	49
30	ArK	$X^2\Sigma^+$	Potassium – argon (1/1)	50
31	ArKr	$X^1\Sigma^+$ (0^+ in Hund's case c notation)	Krypton – argon (1/1)	51
32	ArLi	$X^2\Sigma^+$	Lithium – argon (1/1)	52
33	ArMg	$X^1\Sigma^+$	Magnesium – argon (1/1)	53
34	ArNa	$X^2\Sigma^+$	Sodium – argon (1/1)	55
35	ArNe	$X^1\Sigma^+$ (0^+ in Hund's case c notation)	Argon – neon (1/1).	56
36	ArNe ⁺	$X^2\Sigma^+$	Argon (1+) ion – neon (1/1)	57
37	ArNi		Nickel – argon (1/1), ground state unassigned	58
38	ArSi	$X^3\Sigma^-$	Silicium – argon (1/1)	59
39	ArSn	$X^3\Sigma^-$	Tin – argon (1/1)	60
40	ArXe	$X^1\Sigma^+$ (0^+ in Hund's case c notation)	Xenon – argon (1/1)	61
41	ArZn	$X0^+ (^1\Sigma^+)$	Zinc – argon (1/1)	62
42	Ar ₂	$X^1\Sigma_g^+$ (0_g^+ in Hund's case c notation)	Argon dimer	63
43	Ar ₂ ⁺	$A^2\Sigma_{1/2u}^+$	Diargon (1+) ion	64
44	AsBr	$X^2\Sigma^- (X_10^+, X_21)$	Bromoarsinidene	65
45	AsH	$X^3\Sigma^-$	Arsinidene	66
46	AsI	$X^3\Sigma^- (X_10^+, X_21)$	Iodoarsinidene	67
47	AsP	$X^1\Sigma^+$	Arsenic phosphide	68
48	AuBr	$X^1\Sigma^+$	Gold bromide	69
49	AuCl	$X^1\Sigma^+$	Gold chloride	71
50	AuF	$X^1\Sigma^+$	Gold fluoride	74
51	AuH	$X^1\Sigma^+$	Gold hydride	75
52	AuI	$X^1\Sigma^+$	Gold iodide	77
53	AuO	$X^2\Pi_{1/2}, X^2\Pi_{3/2}$	Gold oxide	78
54	AuO ⁻	$X^1\Sigma^+$	Aurate(1-)	79
55	AuS	$X^2\Pi_{3/2}, X^2\Pi_{1/2}$	Gold sulphide	80
56	AuS ⁻	$X^1\Sigma^+$	Thioxoaurate(1-)	81
57	AuSi	$X^2\Sigma$	Gold silicide	82
58	BBr	$X^1\Sigma^+$	Bromoborane(1)	83
59	BNe	$X^2\Pi$	Boron – neon (1/1)	85
60	BO	$^2\Sigma^+$	Boron oxide	86
61	BRh	$X^1\Sigma^+$	Rhodium boride	87
62	BSi	$X^4\Sigma^-$	Boron silicide	88
63	B ₂	$X^3\Sigma_g^-$	Diboron	89
64	BaF	$^2\Sigma^+$	Barium fluoride	90
65	BaH	$^2\Sigma^+$	Barium hydride	91
66	BaI	$X^2\Sigma^+$	Barium iodide	92
67	BaO	$X^1\Sigma^+$	Barium oxide	93
68	BaS	$X^1\Sigma^+$	Barium sulphide	95
69	Ba ₂	$X^1\Sigma_g^+$	Dibarium	96
70	BeH	$X^2\Sigma^+$	Beryllium hydride	97

71	$\text{BeH}^+ X^1\Sigma^+$	Hydroberyllium(1+) ion	98
72	$\text{BiN} X^1\Sigma^+$	Bismuth nitride	101
73	$\text{BiNa} X^3\Sigma^-$	Sodium – bismuth (1/1)	103
74	$\text{BiO} X_1^2\Pi_i$	Bismuth oxide	104
75	$\text{BiP} X^1\Sigma^+$	Bismuth phosphide	105
76	$\text{BiS} X_1^2\Pi_{1/2}$	Bismuth sulphide	106
77	$\text{Bi}_2 X^1\Sigma_g^+$	Dibismuth	107
78	$\text{BrCl} X^1\Sigma^+ (0^+)$	Bromine chloride	108
79	$\text{BrCl}^+ X^2\Pi_{3/2}$	Bromine chloride(1+) radical ion	110
80	$\text{BrCu} X^1\Sigma^+$	Copper bromide	111
81	$\text{BrF} X^1\Sigma^+ (0^+)$	Bromine fluoride	113
82	$\text{BrH} X^1\Sigma^+ (0^+)$	Hydrogen bromide	115
83	$\text{BrH}^+ X^2\Pi_{3/2}$	Bromoniumyl	119
84	$\text{BrI} X^1\Sigma^+ (0^+)$	Iodine bromide	121
85	$\text{BrI}^+ X^2\Pi_{3/2}$	Bromoiodine(1+) radical ion	127
86	$\text{BrI}^- X^2\Sigma_{1/2}^+$	Bromoiodate(1–)	128
87	$\text{BrIn} X^1\Sigma^+$	Indium bromide	129
88	$\text{BrKr} X1/2$	Krypton bromide	130
89	$\text{BrKr}^- X^1\Sigma^+$	Bromokryptonate(1–)	131
90	$\text{BrLa} X^1\Sigma^+$	Lanthanum bromide	132
91	$\text{BrMg} X^2\Sigma^+$	Magnesium bromide	133
92	$\text{BrN} X^3\Sigma^-$	Nitrogen bromide	134
93	$\text{BrNi} X^2\Pi_{3/2}$	Nickel bromide	135
94	$\text{BrO} X^2\Pi$	Bromine oxide	136
95	$\text{BrO}^+ X^3\Sigma^-$	Bromosyl ion	137
96	$\text{BrSb} X^3\Sigma^-$	Bromostibylene	138
97	$\text{BrSc} X^1\Sigma^+$	Scandium bromide	139
98	$\text{BrSr} X^2\Sigma^+$	Strontium bromide	141
99	$\text{BrTi} X^4\Phi_i (\Omega = 3/2, 5/2, 7/2)$	Titanium bromide	142
100	$\text{BrXe} X1/2$	Xenon bromide	143
101	$\text{BrXe}^- X^1\Sigma^+$	Bromoxenonate(1–)	144
102	$\text{BrY} X^1\Sigma^+$	Yttrium bromide	145
103	$\text{BrYb} X^2\Sigma^+$	Ytterbium bromide	147
104	$\text{Br}_2 X^1\Sigma_g^+ (0_g^+)$	Dibromine	148
105	$\text{CAr} X^3\Sigma^-$	Carbon – argon (1/1)	150
106	$\text{CB} X^4\Sigma^+$	Boron carbide	151
107	$\text{CBr} X^2\Pi_{1/2}$	Bromomethylidyne	152
108	$\text{CCa} X^3\Sigma^-$	Calcium carbide	153
109	$\text{CCl} X^2\Pi$	Chloromethylidyne	154
110	$\text{CCo} X^2\Sigma^+$	Cobalt carbide	155
111	$\text{CCr} X^3\Sigma^-$	Chromium carbide	156
112	$\text{CF} X^2\Pi$	Fluoromethylidyne	157
113	$\text{CFe} X^3\Delta_i$	Iron carbide	158
114	$\text{CH} X^2\Pi$	Methylidyne	159
115	$\text{CH}^+ X^1\Sigma^+$	Methyliumylidene	160
116	$\text{CIr} X^2\Sigma^+$	Iridium carbide	161
117	$\text{CK} X^4\Sigma^-$	Potassium carbide	162
118	$\text{CMo} X^3\Sigma^- (0^+)$	Molybdenum carbide	163
119	$\text{CN} X^2\Sigma^+$	Cyanogen	164

120	CN ⁻	$X^1\Sigma$	Cyanide	165
121	CNa	$X^4\Sigma^-$	Sodium carbide	166
122	CNb	$X^2\Delta_{3/2}$	Niobium carbide	167
123	CNi	$X^1\Sigma^+$	Nickel carbide	168
124	CO ⁺	$X^2\Sigma^+$	Carbon monoxide (1+) ion	170
125	COs	$X^3\Delta^-$	Osmium carbide	171
126	COs ⁺	$X^2\Delta$	Methanetetraylosmium(1+)	172
127	COs ⁻	$X^2\Delta$	Methanetetraylosmate(1-)	173
128	CP	$X^2\Sigma^+$	Phosphinidynemethyl	174
129	CPd	$X^1\Sigma^+$ (0 ⁺)	Palladium carbide	175
130	CPt	$X^1\Sigma^+$	Platinum carbide	177
131	CRh	$X^2\Sigma^+$	Rhodium carbide	178
132	CRu	$X^1\Sigma^+$	Ruthenium carbide	179
133	CS ⁺	$X^2\Sigma^+$	Carbon sulfide (1+) ion	182
134	CSc	$X^2\Pi$	Scandium carbide	183
135	CSi	$X^3\Pi$	Silicon carbide	184
136	CTa	$X^2\Sigma^+$	Tantalum carbide	185
137	CTa ⁺	$X^3\Sigma^+$	Methanetetrayltantalum(1+)	186
138	CTc	$X^4\Sigma^+$	Technetium carbide	187
139	CTi	$X^3\Sigma^+$	Titanium carbide	188
140	CV	$X^4\Delta$	Vanadium carbide	189
141	CW	$X^3\Delta_1$	Tungsten carbide	190
142	CZr	$X^3\Sigma^+$	Zirconium carbide	191
143	C ₂	$X^1\Sigma_g^+$	1,2-Ethynediyl	192
144	C ₂ ⁺	$X^4\Sigma_g^-$	Ethynylium-1-yl	197
145	C ₂ ⁻	$X^2\Sigma_g^+$	Ethynyl (1-) ion	198
146	CaCl	$X^2\Sigma^+$	Calcium chloride	199
147	CaF	$X^2\Sigma^+$	Calcium fluoride	200
148	CaH	$X^2\Sigma^+$	Calcium hydride	201
149	CaKr	$X^1\Sigma^+$	Calcium – krypton (1/1)	202
150	CaKr ⁺	$X^2\Sigma^+$	Calcium (1+) ion – krypton (1/1)	203
151	CaO	$X^1\Sigma^+$	Calcium oxide	204
152	CaS	$X^1\Sigma^+$	Calcium sulfide	206
153	CaXe	$X^1\Sigma^+$	Calcium – xenon (1/1)	207
154	CaXe ⁺	$X^2\Sigma^+$	Calcium (1+) ion – xenon (1/1)	208
155	CdH	$X^2\Sigma^+$	Cadmium hydride	209
156	CdHe	$X0^+ (^1\Sigma^+)$	Cadmium – helium (1/1)	210
157	CdKr	$X0^+ (^1\Sigma^+)$	Cadmium – krypton (1/1)	212
158	CdNe	$X0^+ (^1\Sigma^+)$	Cadmium – neon (1/1)	215
159	CdXe	$X0^+ (^1\Sigma^+)$	Cadmium – xenon (1/1)	217
160	Cd ₂	$X0_g^+ (^1\Sigma_g^+)$	Dicadmium	218
161	ClCo	$X^3\Phi_4$	Cobalt chloride	221
162	ClCr	$X^6\Sigma^+$	Chromium chloride	222
163	ClCu	$X^1\Sigma^+$	Copper chloride	223
164	ClDy	X7.5	Disprosium chloride	226
165	ClF	$X^1\Sigma^+$	Chlorine fluoride	227
166	ClFe	$X^6\Delta_{3/2}$	Iron chloride	230
167	ClGa	$X^1\Sigma^+$	Gallium chloride	231
168	ClGe	$X^2\Pi_r$	Germanium chloride	233

169	$\text{ClH}^+ X^2\Pi_{3/2}$	Chloroniumyl	234
170	$\text{ClH}^{++} X^3\Sigma^-$	Chlorohydrogen (2+) ion	235
171	$\text{ClHf} X^2\Delta_{3/2}$	Hafnium chloride	236
172	$\text{ClHo} X8 (\Omega = 8)$	Holmium chloride	237
173	$\text{ClI} X^1\Sigma^+$	Iodine chloride	238
174	$\text{ClIn} X^1\Sigma^+$	Indium chloride	240
175	$\text{KCl} X^1\Sigma^+$	Potassium chloride	242
176	$\text{ClKr} X1/2$	Krypton chloride	244
177	$\text{ClKr}^- X^1\Sigma^+$	Chlorokryptonate(1-)	245
178	$\text{ClLa} X^1\Sigma^+$	Lanthanum chloride	246
179	$\text{CLu} X^1\Sigma^+$	Lutetium chloride	248
180	$\text{ClMg} X^2\Sigma^+$	Magnesium chloride	250
181	$\text{ClMn} X^7\Sigma^+$	Manganese chloride	251
182	$\text{ClN} X^3\Sigma^-$	Nitrogen chloride	252
183	$\text{ClNa} X^1\Sigma^+$	Sodium chloride	253
184	$\text{ClNb} X^5\Pi$	Niobium chloride	255
185	$\text{ClNi} X^2\Pi_{3/2}$	Nickel chloride	256
186	$\text{ClO} X^2\Pi$	Chlorine oxide	257
187	$\text{ClPb} X^2\Pi_i$	Lead chloride	258
188	$\text{ClRb} X^1\Sigma^+$	Rubidium chloride	259
189	$\text{ClRh} X^3\Pi_i$	Rhodium chloride	262
190	$\text{ClSb} X^3\Sigma^-$	Chlorostibylene	263
191	$\text{ClSc} X^1\Sigma^+$	Scandium chloride	264
192	$\text{ClSi} X^2\Pi$	Chlorosilyldyne	267
193	$\text{ClSi}^+ X^1\Sigma^+$	Chlorosilyliumylidene	268
194	$\text{ClTa} X(^3\Sigma_0^+, ^3\Phi_2)$	Tantalum chloride	270
195	$\text{ClTi} X^4\Phi_i$	Titanium chloride	271
196	$\text{ClTi}^+ X^3\Phi_r$	Chlorotitanium(1+) ion	272
197	$\text{ClV} X^5\Delta$	Vanadium chloride	273
198	$\text{ClXe} X1/2$	Xenon chloride	274
199	$\text{ClXe}^- X^1\Sigma^+$	Chloroxenonate(1-)	275
200	$\text{ClY} X^1\Sigma^+$	Yttrium chloride	276
201	$\text{ClYb} X^2\Sigma^+$	Ytterbium chloride	278
202	$\text{ClZr} X^2\Delta$	Zirconium chloride	279
203	$\text{Cl}_2 X^1\Sigma_g^+$	Dichlorine	280
204	$\text{Cl}_2^+ X^2\Pi_g$	Dichlorine(1+) ion	283

Note: The data for CO, CS, and ClH are included in subvolume II/29A2.