

Table 1: Space group information.

ID	tag			Schönflies	international	setting	crystal	PG
1	C1^1	SG:1	1	C_1^1	$P1$		triclinic	C_1
2	Ci^1	SG:2	2	C_i^1	$P\bar{1}$		triclinic	C_i
3	C2^1	SG:3	3	C_2^1	$P2$	b-axis	monoclinic	C_2
4	C2^2	SG:4	4	C_2^2	$P2_1$	b-axis	monoclinic	C_2
5	C2^3	SG:5	5	C_2^3	$C2$	b-axis	monoclinic	C_2
6	Cs^1	SG:6	6	C_s^1	Pm	b-axis	monoclinic	C_s
7	Cs^2	SG:7	7	C_s^2	Pc	b-axis	monoclinic	C_s
8	Cs^3	SG:8	8	C_s^3	Cm	b-axis	monoclinic	C_s
9	Cs^4	SG:9	9	C_s^4	Cc	b-axis	monoclinic	C_s
10	C2h^1	SG:10	10	C_{2h}^1	$P2/m$	b-axis	monoclinic	C_{2h}
11	C2h^2	SG:11	11	C_{2h}^2	$P2_1/m$	b-axis	monoclinic	C_{2h}
12	C2h^3	SG:12	12	C_{2h}^3	$C2/m$	b-axis	monoclinic	C_{2h}
13	C2h^4	SG:13	13	C_{2h}^4	$P2/c$	b-axis	monoclinic	C_{2h}
14	C2h^5	SG:14	14	C_{2h}^5	$P2_1/c$	b-axis	monoclinic	C_{2h}
15	C2h^6	SG:15	15	C_{2h}^6	$C2/c$	b-axis	monoclinic	C_{2h}
16	D2^1	SG:16	16	D_2^1	$P222$		orthorhombic	D_2
17	D2^2	SG:17	17	D_2^2	$P222_1$		orthorhombic	D_2
18	D2^3	SG:18	18	D_2^3	$P2_12_12$		orthorhombic	D_2
19	D2^4	SG:19	19	D_2^4	$P2_12_12_1$		orthorhombic	D_2
20	D2^5	SG:20	20	D_2^5	$C222_1$		orthorhombic	D_2
21	D2^6	SG:21	21	D_2^6	$C222$		orthorhombic	D_2
22	D2^7	SG:22	22	D_2^7	$F222$		orthorhombic	D_2
23	D2^8	SG:23	23	D_2^8	$I222$		orthorhombic	D_2
24	D2^9	SG:24	24	D_2^9	$I2_12_12_1$		orthorhombic	D_2
25	C2v^1	SG:25	25	C_{2v}^1	$Pmm2$		orthorhombic	C_{2v}
26	C2v^2	SG:26	26	C_{2v}^2	$Pmc2_1$		orthorhombic	C_{2v}
27	C2v^3	SG:27	27	C_{2v}^3	$Pcc2$		orthorhombic	C_{2v}
28	C2v^4	SG:28	28	C_{2v}^4	$Pma2$		orthorhombic	C_{2v}
29	C2v^5	SG:29	29	C_{2v}^5	$Pca2_1$		orthorhombic	C_{2v}
30	C2v^6	SG:30	30	C_{2v}^6	$Pnc2$		orthorhombic	C_{2v}
31	C2v^7	SG:31	31	C_{2v}^7	$Pmn2_1$		orthorhombic	C_{2v}
32	C2v^8	SG:32	32	C_{2v}^8	$Pba2$		orthorhombic	C_{2v}
33	C2v^9	SG:33	33	C_{2v}^9	$Pna2_1$		orthorhombic	C_{2v}
34	C2v^10	SG:34	34	C_{2v}^{10}	$Pnn2$		orthorhombic	C_{2v}
35	C2v^11	SG:35	35	C_{2v}^{11}	$Cmm2$		orthorhombic	C_{2v}
36	C2v^12	SG:36	36	C_{2v}^{12}	$Cmc2_1$		orthorhombic	C_{2v}
37	C2v^13	SG:37	37	C_{2v}^{13}	$Ccc2$		orthorhombic	C_{2v}
38	C2v^14	SG:38	38	C_{2v}^{14}	$Amm2$		orthorhombic	C_{2v}
39	C2v^15	SG:39	39	C_{2v}^{15}	$Aem2$		orthorhombic	C_{2v}
40	C2v^16	SG:40	40	C_{2v}^{16}	$Ama2$		orthorhombic	C_{2v}
41	C2v^17	SG:41	41	C_{2v}^{17}	$Aea2$		orthorhombic	C_{2v}
42	C2v^18	SG:42	42	C_{2v}^{18}	$Fmm2$		orthorhombic	C_{2v}
43	C2v^19	SG:43	43	C_{2v}^{19}	$Fdd2$		orthorhombic	C_{2v}

continued ...

Table 1

ID	tag			Schönflies	international	setting	crystal	PG
44	C2v^20	SG:44	44	C_{2v}^{20}	$Imm2$		orthorhombic	C_{2v}
45	C2v^21	SG:45	45	C_{2v}^{21}	$Iba2$		orthorhombic	C_{2v}
46	C2v^22	SG:46	46	C_{2v}^{22}	$Ima2$		orthorhombic	C_{2v}
47	D2h^1	SG:47	47	D_{2h}^1	$Pmmm$		orthorhombic	D_{2h}
48	D2h^2	SG:48	48	D_{2h}^2	$Pnnn$		orthorhombic	D_{2h}
49	D2h^3	SG:49	49	D_{2h}^3	$Pccm$		orthorhombic	D_{2h}
50	D2h^4	SG:50	50	D_{2h}^4	$Pban$		orthorhombic	D_{2h}
51	D2h^5	SG:51	51	D_{2h}^5	$Pmma$		orthorhombic	D_{2h}
52	D2h^6	SG:52	52	D_{2h}^6	$Pnna$		orthorhombic	D_{2h}
53	D2h^7	SG:53	53	D_{2h}^7	$Pmna$		orthorhombic	D_{2h}
54	D2h^8	SG:54	54	D_{2h}^8	$Pcca$		orthorhombic	D_{2h}
55	D2h^9	SG:55	55	D_{2h}^9	$Pbam$		orthorhombic	D_{2h}
56	D2h^10	SG:56	56	D_{2h}^{10}	$Pccn$		orthorhombic	D_{2h}
57	D2h^11	SG:57	57	D_{2h}^{11}	$Pbcm$		orthorhombic	D_{2h}
58	D2h^12	SG:58	58	D_{2h}^{12}	$Pnnm$		orthorhombic	D_{2h}
59	D2h^13	SG:59	59	D_{2h}^{13}	$Pmmn$		orthorhombic	D_{2h}
60	D2h^14	SG:60	60	D_{2h}^{14}	$Pbcn$		orthorhombic	D_{2h}
61	D2h^15	SG:61	61	D_{2h}^{15}	$Pbca$		orthorhombic	D_{2h}
62	D2h^16	SG:62	62	D_{2h}^{16}	$Pnma$		orthorhombic	D_{2h}
63	D2h^17	SG:63	63	D_{2h}^{17}	$Cmcm$		orthorhombic	D_{2h}
64	D2h^18	SG:64	64	D_{2h}^{18}	$Cmce$		orthorhombic	D_{2h}
65	D2h^19	SG:65	65	D_{2h}^{19}	$Cmmm$		orthorhombic	D_{2h}
66	D2h^20	SG:66	66	D_{2h}^{20}	$Cccm$		orthorhombic	D_{2h}
67	D2h^21	SG:67	67	D_{2h}^{21}	$Cmme$		orthorhombic	D_{2h}
68	D2h^22	SG:68	68	D_{2h}^{22}	$Ccce$		orthorhombic	D_{2h}
69	D2h^23	SG:69	69	D_{2h}^{23}	$Fmmm$		orthorhombic	D_{2h}
70	D2h^24	SG:70	70	D_{2h}^{24}	$Fddd$		orthorhombic	D_{2h}
71	D2h^25	SG:71	71	D_{2h}^{25}	Imm		orthorhombic	D_{2h}
72	D2h^26	SG:72	72	D_{2h}^{26}	$Ibam$		orthorhombic	D_{2h}
73	D2h^27	SG:73	73	D_{2h}^{27}	$Ibca$		orthorhombic	D_{2h}
74	D2h^28	SG:74	74	D_{2h}^{28}	$Imma$		orthorhombic	D_{2h}
75	C4^1	SG:75	75	C_4^1	$P4$		tetragonal	C_4
76	C4^2	SG:76	76	C_4^2	$P4_1$		tetragonal	C_4
77	C4^3	SG:77	77	C_4^3	$P4_2$		tetragonal	C_4
78	C4^4	SG:78	78	C_4^4	$P4_3$		tetragonal	C_4
79	C4^5	SG:79	79	C_4^5	$I4$		tetragonal	C_4
80	C4^6	SG:80	80	C_4^6	$I4_1$		tetragonal	C_4
81	S4^1	SG:81	81	S_4^1	$P\bar{4}$		tetragonal	S_4
82	S4^2	SG:82	82	S_4^2	$I\bar{4}$		tetragonal	S_4
83	C4h^1	SG:83	83	C_{4h}^1	$P4/m$		tetragonal	C_{4h}
84	C4h^2	SG:84	84	C_{4h}^2	$P4_2/m$		tetragonal	C_{4h}
85	C4h^3	SG:85	85	C_{4h}^3	$P4/n$		tetragonal	C_{4h}
86	C4h^4	SG:86	86	C_{4h}^4	$P4_2/n$		tetragonal	C_{4h}
87	C4h^5	SG:87	87	C_{4h}^5	$I4/m$		tetragonal	C_{4h}

continued ...

Table 1

ID	tag			Schönflies	international	setting	crystal	PG
88	C4h^6	SG:88	88	C_{4h}^6	$I4_1/a$		tetragonal	C_{4h}
89	D4^1	SG:89	89	D_4^1	$P422$		tetragonal	D_4
90	D4^2	SG:90	90	D_4^2	$P4_212$		tetragonal	D_4
91	D4^3	SG:91	91	D_4^3	$P4_122$		tetragonal	D_4
92	D4^4	SG:92	92	D_4^4	$P4_12_12$		tetragonal	D_4
93	D4^5	SG:93	93	D_4^5	$P4_222$		tetragonal	D_4
94	D4^6	SG:94	94	D_4^6	$P4_22_12$		tetragonal	D_4
95	D4^7	SG:95	95	D_4^7	$P4_322$		tetragonal	D_4
96	D4^8	SG:96	96	D_4^8	$P4_32_12$		tetragonal	D_4
97	D4^9	SG:97	97	D_4^9	$I422$		tetragonal	D_4
98	D4^10	SG:98	98	D_4^{10}	$I4_122$		tetragonal	D_4
99	C4v^1	SG:99	99	C_{4v}^1	$P4mm$		tetragonal	C_{4v}
100	C4v^2	SG:100	100	C_{4v}^2	$P4bm$		tetragonal	C_{4v}
101	C4v^3	SG:101	101	C_{4v}^3	$P4_2cm$		tetragonal	C_{4v}
102	C4v^4	SG:102	102	C_{4v}^4	$P4_2nm$		tetragonal	C_{4v}
103	C4v^5	SG:103	103	C_{4v}^5	$P4cc$		tetragonal	C_{4v}
104	C4v^6	SG:104	104	C_{4v}^6	$P4nc$		tetragonal	C_{4v}
105	C4v^7	SG:105	105	C_{4v}^7	$P4_2mc$		tetragonal	C_{4v}
106	C4v^8	SG:106	106	C_{4v}^8	$P4_2bc$		tetragonal	C_{4v}
107	C4v^9	SG:107	107	C_{4v}^9	$I4mm$		tetragonal	C_{4v}
108	C4v^10	SG:108	108	C_{4v}^{10}	$I4cm$		tetragonal	C_{4v}
109	C4v^11	SG:109	109	C_{4v}^{11}	$I4_1md$		tetragonal	C_{4v}
110	C4v^12	SG:110	110	C_{4v}^{12}	$I4_1cd$		tetragonal	C_{4v}
111	D2d^1	SG:111	111	D_{2d}^1	$P\bar{4}2m$		tetragonal	D_{2d}
112	D2d^2	SG:112	112	D_{2d}^2	$P\bar{4}2c$		tetragonal	D_{2d}
113	D2d^3	SG:113	113	D_{2d}^3	$P\bar{4}2_1m$		tetragonal	D_{2d}
114	D2d^4	SG:114	114	D_{2d}^4	$P\bar{4}2_1c$		tetragonal	D_{2d}
115	D2d^5	SG:115	115	D_{2d}^5	$P\bar{4}m2$		tetragonal	$D_{2d}(1)$
116	D2d^6	SG:116	116	D_{2d}^6	$P\bar{4}c2$		tetragonal	$D_{2d}(1)$
117	D2d^7	SG:117	117	D_{2d}^7	$P\bar{4}b2$		tetragonal	$D_{2d}(1)$
118	D2d^8	SG:118	118	D_{2d}^8	$P\bar{4}n2$		tetragonal	$D_{2d}(1)$
119	D2d^9	SG:119	119	D_{2d}^9	$I\bar{4}m2$		tetragonal	$D_{2d}(1)$
120	D2d^10	SG:120	120	D_{2d}^{10}	$I\bar{4}c2$		tetragonal	$D_{2d}(1)$
121	D2d^11	SG:121	121	D_{2d}^{11}	$I\bar{4}2m$		tetragonal	D_{2d}
122	D2d^12	SG:122	122	D_{2d}^{12}	$I\bar{4}2d$		tetragonal	D_{2d}
123	D4h^1	SG:123	123	D_{4h}^1	$P4/mmm$		tetragonal	D_{4h}
124	D4h^2	SG:124	124	D_{4h}^2	$P4/mcc$		tetragonal	D_{4h}
125	D4h^3	SG:125	125	D_{4h}^3	$P4/nbm$		tetragonal	D_{4h}
126	D4h^4	SG:126	126	D_{4h}^4	$P4/nnc$		tetragonal	D_{4h}
127	D4h^5	SG:127	127	D_{4h}^5	$P4/mbm$		tetragonal	D_{4h}
128	D4h^6	SG:128	128	D_{4h}^6	$P4/mnc$		tetragonal	D_{4h}
129	D4h^7	SG:129	129	D_{4h}^7	$P4/nmm$		tetragonal	D_{4h}
130	D4h^8	SG:130	130	D_{4h}^8	$P4/ncc$		tetragonal	D_{4h}
131	D4h^9	SG:131	131	D_{4h}^9	$P4_2/mmc$		tetragonal	D_{4h}

continued ...

Table 1

ID	tag		Schönflies	international	setting	crystal	PG
132	D4h^10	SG:132	132	D_{4h}^{10}	$P4_2/mcm$	tetragonal	D_{4h}
133	D4h^11	SG:133	133	D_{4h}^{11}	$P4_2/nbc$	tetragonal	D_{4h}
134	D4h^12	SG:134	134	D_{4h}^{12}	$P4_2/nnm$	tetragonal	D_{4h}
135	D4h^13	SG:135	135	D_{4h}^{13}	$P4_2/mbc$	tetragonal	D_{4h}
136	D4h^14	SG:136	136	D_{4h}^{14}	$P4_2/mnm$	tetragonal	D_{4h}
137	D4h^15	SG:137	137	D_{4h}^{15}	$P4_2/nmc$	tetragonal	D_{4h}
138	D4h^16	SG:138	138	D_{4h}^{16}	$P4_2/ncm$	tetragonal	D_{4h}
139	D4h^17	SG:139	139	D_{4h}^{17}	$I4/mmm$	tetragonal	D_{4h}
140	D4h^18	SG:140	140	D_{4h}^{18}	$I4/mcm$	tetragonal	D_{4h}
141	D4h^19	SG:141	141	D_{4h}^{19}	$I4_1/amd$	tetragonal	D_{4h}
142	D4h^20	SG:142	142	D_{4h}^{20}	$I4_1/acd$	tetragonal	D_{4h}
143	C3^1	SG:143	143	C_3^1	$P3$	trigonal	C_3
144	C3^2	SG:144	144	C_3^2	$P3_1$	trigonal	C_3
145	C3^3	SG:145	145	C_3^3	$P3_2$	trigonal	C_3
146	C3^4	SG:146	146	C_3^4	$R3$	trigonal	C_3
147	C3i^1	SG:147	147	C_{3i}^1	$P\bar{3}$	trigonal	C_{3i}
148	C3i^2	SG:148	148	C_{3i}^2	$R\bar{3}$	trigonal	C_{3i}
149	D3^1	SG:149	149	D_3^1	$P312$	trigonal	$D_3(1)$
150	D3^2	SG:150	150	D_3^2	$P321$	trigonal	D_3
151	D3^3	SG:151	151	D_3^3	$P3_112$	trigonal	$D_3(1)$
152	D3^4	SG:152	152	D_3^4	$P3_121$	trigonal	D_3
153	D3^5	SG:153	153	D_3^5	$P3_212$	trigonal	$D_3(1)$
154	D3^6	SG:154	154	D_3^6	$P3_221$	trigonal	D_3
155	D3^7	SG:155	155	D_3^7	$R32$	trigonal	D_3
156	C3v^1	SG:156	156	C_{3v}^1	$P3m1$	trigonal	C_{3v}
157	C3v^2	SG:157	157	C_{3v}^2	$P31m$	trigonal	$C_{3v}(1)$
158	C3v^3	SG:158	158	C_{3v}^3	$P3c1$	trigonal	C_{3v}
159	C3v^4	SG:159	159	C_{3v}^4	$P31c$	trigonal	$C_{3v}(1)$
160	C3v^5	SG:160	160	C_{3v}^5	$R3m$	trigonal	C_{3v}
161	C3v^6	SG:161	161	C_{3v}^6	$R3c$	trigonal	C_{3v}
162	D3d^1	SG:162	162	D_{3d}^1	$P\bar{3}1m$	trigonal	$D_{3d}(1)$
163	D3d^2	SG:163	163	D_{3d}^2	$P\bar{3}1c$	trigonal	$D_{3d}(1)$
164	D3d^3	SG:164	164	D_{3d}^3	$P\bar{3}m1$	trigonal	D_{3d}
165	D3d^4	SG:165	165	D_{3d}^4	$P\bar{3}c1$	trigonal	D_{3d}
166	D3d^5	SG:166	166	D_{3d}^5	$R\bar{3}m$	trigonal	D_{3d}
167	D3d^6	SG:167	167	D_{3d}^6	$R\bar{3}c$	trigonal	D_{3d}
168	C6^1	SG:168	168	C_6^1	$P6$	hexagonal	C_6
169	C6^2	SG:169	169	C_6^2	$P6_1$	hexagonal	C_6
170	C6^3	SG:170	170	C_6^3	$P6_5$	hexagonal	C_6
171	C6^4	SG:171	171	C_6^4	$P6_2$	hexagonal	C_6
172	C6^5	SG:172	172	C_6^5	$P6_4$	hexagonal	C_6
173	C6^6	SG:173	173	C_6^6	$P6_3$	hexagonal	C_6
174	C3h^1	SG:174	174	C_{3h}^1	$P\bar{6}$	hexagonal	C_{3h}
175	C6h^1	SG:175	175	C_{6h}^1	$P6/m$	hexagonal	C_{6h}

continued ...

Table 1

ID	tag			Schönflies	international	setting	crystal	PG
176	C6h^2	SG:176	176	C_{6h}^2	$P6_3/m$		hexagonal	C_{6h}
177	D6^1	SG:177	177	D_6^1	$P622$		hexagonal	D_6
178	D6^2	SG:178	178	D_6^2	$P6_{12}2$		hexagonal	D_6
179	D6^3	SG:179	179	D_6^3	$P6_{52}2$		hexagonal	D_6
180	D6^4	SG:180	180	D_6^4	$P6_{22}2$		hexagonal	D_6
181	D6^5	SG:181	181	D_6^5	$P6_{42}2$		hexagonal	D_6
182	D6^6	SG:182	182	D_6^6	$P6_{32}2$		hexagonal	D_6
183	C6v^1	SG:183	183	C_{6v}^1	$P6mm$		hexagonal	C_{6v}
184	C6v^2	SG:184	184	C_{6v}^2	$P6cc$		hexagonal	C_{6v}
185	C6v^3	SG:185	185	C_{6v}^3	$P6_3cm$		hexagonal	C_{6v}
186	C6v^4	SG:186	186	C_{6v}^4	$P6_3mc$		hexagonal	C_{6v}
187	D3h^1	SG:187	187	D_{3h}^1	$P\bar{6}m2$		hexagonal	D_{3h}
188	D3h^2	SG:188	188	D_{3h}^2	$P\bar{6}c2$		hexagonal	D_{3h}
189	D3h^3	SG:189	189	D_{3h}^3	$P\bar{6}2m$		hexagonal	$D_{3h}(1)$
190	D3h^4	SG:190	190	D_{3h}^4	$P\bar{6}2c$		hexagonal	$D_{3h}(1)$
191	D6h^1	SG:191	191	D_{6h}^1	$P6/mmm$		hexagonal	D_{6h}
192	D6h^2	SG:192	192	D_{6h}^2	$P6/mcc$		hexagonal	D_{6h}
193	D6h^3	SG:193	193	D_{6h}^3	$P6_3/mcm$		hexagonal	D_{6h}
194	D6h^4	SG:194	194	D_{6h}^4	$P6_3/mmc$		hexagonal	D_{6h}
195	T^1	SG:195	195	T^1	$P23$		cubic	T
196	T^2	SG:196	196	T^2	$F23$		cubic	T
197	T^3	SG:197	197	T^3	$I23$		cubic	T
198	T^4	SG:198	198	T^4	$P2_13$		cubic	T
199	T^5	SG:199	199	T^5	$I2_13$		cubic	T
200	Th^1	SG:200	200	T_h^1	$Pm\bar{3}$		cubic	T_h
201	Th^2	SG:201	201	T_h^2	$Pn\bar{3}$		cubic	T_h
202	Th^3	SG:202	202	T_h^3	$Fm\bar{3}$		cubic	T_h
203	Th^4	SG:203	203	T_h^4	$Fd\bar{3}$		cubic	T_h
204	Th^5	SG:204	204	T_h^5	$Im\bar{3}$		cubic	T_h
205	Th^6	SG:205	205	T_h^6	$Pa\bar{3}$		cubic	T_h
206	Th^7	SG:206	206	T_h^7	$Ia\bar{3}$		cubic	T_h
207	O^1	SG:207	207	O^1	$P432$		cubic	O
208	O^2	SG:208	208	O^2	$P4_232$		cubic	O
209	O^3	SG:209	209	O^3	$F432$		cubic	O
210	O^4	SG:210	210	O^4	$F4_132$		cubic	O
211	O^5	SG:211	211	O^5	$I432$		cubic	O
212	O^6	SG:212	212	O^6	$P4_332$		cubic	O
213	O^7	SG:213	213	O^7	$P4_132$		cubic	O
214	O^8	SG:214	214	O^8	$I4_132$		cubic	O
215	Td^1	SG:215	215	T_d^1	$P\bar{4}3m$		cubic	T_d
216	Td^2	SG:216	216	T_d^2	$F\bar{4}3m$		cubic	T_d
217	Td^3	SG:217	217	T_d^3	$I\bar{4}3m$		cubic	T_d
218	Td^4	SG:218	218	T_d^4	$P\bar{4}3n$		cubic	T_d
219	Td^5	SG:219	219	T_d^5	$F\bar{4}3c$		cubic	T_d

continued ...

Table 1

ID	tag		Schönflies	international	setting	crystal	PG
220	Td^6	SG:220	220	T_d^6	$I\bar{4}3d$	cubic	T_d
221	Oh^1	SG:221	221	O_h^1	$Pm\bar{3}m$	cubic	O_h
222	Oh^2	SG:222	222	O_h^2	$Pn\bar{3}n$	cubic	O_h
223	Oh^3	SG:223	223	O_h^3	$Pm\bar{3}n$	cubic	O_h
224	Oh^4	SG:224	224	O_h^4	$Pn\bar{3}m$	cubic	O_h
225	Oh^5	SG:225	225	O_h^5	$Fm\bar{3}m$	cubic	O_h
226	Oh^6	SG:226	226	O_h^6	$Fm\bar{3}c$	cubic	O_h
227	Oh^7	SG:227	227	O_h^7	$Fd\bar{3}m$	cubic	O_h
228	Oh^8	SG:228	228	O_h^8	$Fd\bar{3}c$	cubic	O_h
229	Oh^9	SG:229	229	O_h^9	$Im\bar{3}m$	cubic	O_h
230	Oh^10	SG:230	230	O_h^{10}	$Ia\bar{3}d$	cubic	O_h