

the whole set of 00 l reflexions and can be ruled out. I and IV give alternating signs for consecutive reflexions in the set and were considered unlikely; moreover, IV corresponds to the trivial solution. Only V and VIII of the four combinations left gave models with a satisfactory distribution of peak heights in the E maps and no ghost peaks. The model from VIII proved to be correct.

Table 4. Signs of some 00 l reflexions for various sign combinations in starting set A1

	I	II	III	IV	V	VI	VII	VIII
	$a = +$	$a = +$	$a = +$	$a = +$	$a = -$	$a = -$	$a = -$	$a = -$
	$b = +$	$b = +$	$b = -$	$b = -$	$b = +$	$b = +$	$b = -$	$b = -$
00 l	$c = +$	$c = -$	$c = +$	$c = -$	$c = +$	$c = -$	$c = +$	$c = -$
$l = 34$	+	+	+	+	-	-	-	-
35	-	+	+	-	+	-	-	+
36	+	-	-	+	+	-	-	+
37	-	-	-	-	-	-	-	-
38	+	-	-	+	+	-	-	+
39	-	+	+	-	+	-	-	+
40	+	+	+	+	-	-	-	-
41	-	-	-	-	-	-	-	-
42	+	-	-	+	+	-	-	+
43	-	+	+	-	+	-	-	+
44	+	+	+	+	-	-	-	-

Conclusions

Intersymbolic relations are of no significance in selecting the correct sign combination in a chosen starting set in $P\bar{1}$.

When incorrect signs have been included in the data, they may cause a very rapid propagation of more errors

during the symbolic-addition procedure. It may therefore prove advantageous to break off the Σ_2 process at an early stage and calculate E maps with a small number of terms. For three cases examined, E maps were calculated with the 50 structure factors signed in the first stages by Σ_2 . They were found to contain as much or even significantly more correct information than maps based on all E 's above some arbitrary limit, e.g. 1.2. It is implied that if incorrect signs enter into the data at a very early stage, even reduced E maps may contain too many erroneous features.

Discrimination between probable and less probable sign models may be aided by the use of structural information. A rather crude application of structural knowledge is shown as an example from the work on a chain structure. More refined methods based on these principles could certainly be of great value, in particular with structures giving heavy overlap in Patterson space.

References

- BÜRGI, H. B. & DUNITZ, J. D. (1971). *Acta Cryst.* **A27**, 117-119.
 COCHRAN, W. & WOOLFSON, M. M. (1955). *Acta Cryst.* **8**, 1-12.
 HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem. I. The Centrosymmetric Crystal*, A.C.A. Monograph No. 3. Pittsburgh: Polycrystal Book Service.
 HJORTÅS, J. (1969). Tek. Rapp. 07-R11-69. Inst. for Røntgenteknikk, NTH, Trondheim, Norway.
 HJORTÅS, J. (1972). *Acta Cryst.* **B28**, 2252-2259.
 MO, F. (1971). Unpublished results.
 RØ, G. & SØRUM, H. (1972). *Acta Cryst.* **B28**, 1677-1684.

Acta Cryst. (1973). **A29**, 362

A Complete Catalogue of Polyhedra with Eight or Fewer Vertices

BY DOYLE BRITTON* AND J. D. DUNITZ

Laboratory for Organic Chemistry, Federal Institute of Technology, 8006 Zurich, Switzerland

(Received 29 January 1973; accepted 30 January 1973)

All non-isomorphic convex polyhedra with 4, 5, 6, 7 and 8 vertices are listed. The relationships within each class are described.

In the course of an attempt to describe in a systematic way the coordination of eight ligand atoms around a central atom with no symmetry restrictions, we encountered the problem of enumerating all possible non-isomorphic convex polyhedra with eight vertices. According to Alexandrow (1958) the number $N(n)$ of

polyhedra with n vertices is: $N(4)=1$, $N(5)=2$, $N(6)=7$, $N(7)=34$, $N(8)=257$, but we were unable to find any publication in which these polyhedra are described. Grace (1965) has determined by computer search all polyhedra with up to eleven faces with the restriction that only three edges meet at each vertex. The duals of these polyhedra are the polyhedra with up to eleven vertices with the restriction that all faces are triangular; these, however, are only a small fraction of the

* Permanent address: Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455, U.S.A.

total. Since we could not find the complete list, we decided to make it. We report the results here and shall discuss some of the possible applications elsewhere.

The preparation of the list was briefly as follows: beginning with the tetrahedron, the only polyhedron of order 4, all completely triangulated convex polyhedra (*i.e.* only triangular faces permitted) of order $n+1$ were generated by adding an extra vertex in all possible ways and completing the extra triangles. Our

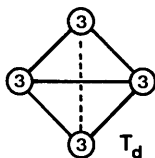


Fig. 1. The tetrahedron – the only polyhedron with four vertices.

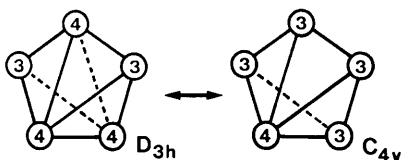


Fig. 2. The two polyhedra with five vertices.

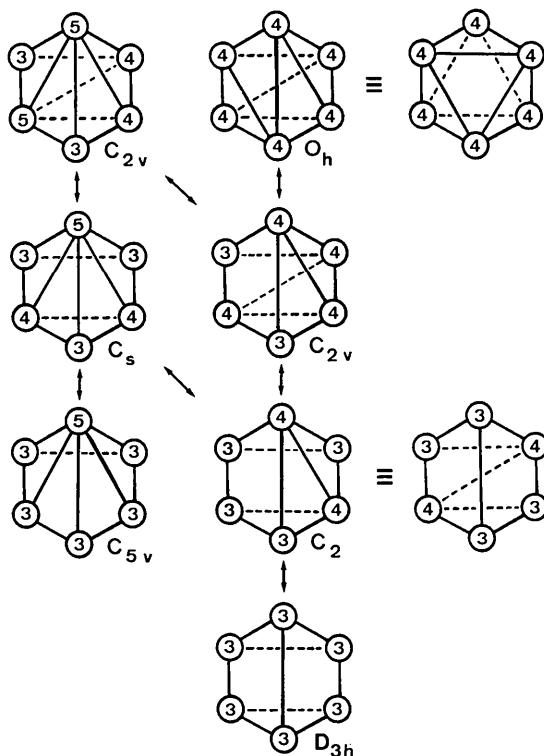


Fig. 3. The seven polyhedra with six vertices: these are shown in the left and centre columns. The right-hand column shows alternative representations for some of the polyhedra in the centre column. The arrows indicate relationship by the removal or addition of an edge.

results agreed with Grace's list. The list for order n was then expanded by removing one edge at a time to produce first quadrilateral faces, then pentagonal faces or pairs of quadrilateral faces, *etc.* This expansion process was continued until further removal of edges would necessarily lead to vertices associated with less than three edges or to non-convex polyhedra with two faces sharing non-adjacent vertices. After elimination of the extensive replications this process finally led to the complete list for order n .

The tetrahedron is the only polyhedron with four vertices. We represent it as in Fig. 1. The circles correspond to vertices, the numbers in the circles give the number of edges that terminate at that vertex, and the lines represent edges, dotted lines corresponding to edges that would be hidden if the faces were opaque. The numbers are redundant but they make the more complicated figures easier to follow and also guard against drawing and copying errors. Although all tetrahedra are equivalent in a topological sense, and no symmetry is required, the maximum possible symmetry of the polyhedron is also given.

We shall represent all of the polyhedra in the same way. That is, we shall show all the vertices on the perimeter of a polygon of order n , with the appropriate diagonals. This corresponds to tracing a Hamilton circuit (a closed path that visits each vertex once and only once) for each polyhedron. In general there is more than one such circuit possible so that our representation is not unique. There are many other ways of drawing such polyhedra, and indeed, for any given polyhedron some other way is likely to be preferred.

Table 1. The relationships among the polyhedra with seven vertices

The polyhedra listed by number (see Fig. 4) in the first column can be generated by removing the appropriate edge from the immediately following polyhedra or by adding a diagonal across the appropriate quadrilateral, pentagonal, or hexagonal faces of the polyhedra in the second list.

I	REMOVE EDGE FROM	ADD EDGE TO
1	0	6 9
2	0	6 7 11
3	0	7 8 10 12
4	0	9 12 13
5	0	11 13
6	1 2	14 17 22
7	2 3	14 16 17 18 19
8	3	15 18 20
9	1 4	17 21 22
10	2 5	15 22
11	2 5	15 22
12	3 4	15 17 19 20 24
13	4 5	15 19 21 22 23 24
14	6 7 10	25 26
15	8 12 13	26 27
16	7	25 28
17	6 7 9 12	26 30
18	7 8	25 31
19	7 11 12 13	26 28 30 31
20	8 10 12 12	26 27 31 32
21	9 13	28 29 30
22	6 9 11 13	26 30
23	13	27 29 30
24	12 13	27 30 31
25	14 16	0
26	14 15 17 18 19 20 22	33
27	15 20 23 24	33
28	16 17 19 21	34
29	21 23	34
30	17 19 21 22 23 24	33 34
31	18 19 20 24	33
32	20	33
33	26 27 30 31 32	0
34	28 29 30	0

Table 2. *The relationships among the polyhedra with eight vertices*

The explanation of the table is the same as for Table 1 except refer to Fig. 5 instead of Fig. 4.

1	REMOVE EDGE FROM	ADD EDGE TO	1	REMOVE EDGE FROM	ADD EDGE TO
1	0	16	129	53 54 57 65 83	203 204
2	0	29	130	56 61 65 84 110	204 205
3	0	31	131	60 64 82 123	205
4	0	34	132	54 65 66 83	203 209
5	0	35	133	52 58 67 87	201 202 208
6	0	38	134	54 67 70 74 78 95	204 206 219
7	0	40	135	54 55 67 60 87 89 91	206 209 216
8	0	41	136	55 75 104 106	207 215
9	0	42	137	53 62 71 84 88	208 218
10	0	44	138	54 62 84 85 86 90 109	204 207 216 219
11	0	48	139	55 62 76 92 93 110 111	209 213 215 220
12	0	49	140	57 61 77 86 88 95 97	204 211 214 217
13	0	50	141	57 58 74 75 87 94 100	204 207 214 217
14	0	51	142	55 64 81 95 103 118 119	213 215 216 226
15	2	55	143	62 84 121 122 125 126	215 216 218 222 225
16	1 8	55	144	60 60 91 95 101 102 114	205 205 219 223
17	2 3	55	145	58 63 79 90 100 118 120	210 212 217 227
18	4 5	53	146	58 60 91 97 104 107 116	205 212 214 225
19	4 5	54	147	59 70 89 101 110 123	206 212 220 224
20	2 5	54	148	50 64 102 104 112 117 126	205 207 218 225 227
21	2 5	54	149	59 63 94 109 112 126 127	207 212 221 224 226
22	5 6	54	150	60 62 105 113 116 127 124	208 208 219 220 225
23	2 11	54	151	61 61 105 113 114 116 121	205 208 214 223 224
24	2 8	59	152	61 63 105 106 115 120 126	208 211 217 221 224
25	3 11	58	153	62 64 123 121 122 125 126	205 208 213 215 216 218 222 225
26	5	76	154	64 108 119 127	207 213 222 227
27	5 7	59	155	63 64 113 125 128	208 226 227
28	5 7	56	156	65 69 70 71 77 96	204 227 228
29	2 12	56	157	65 68 69 72 86 96	209 228 230
30	3 9	72	158	66 67 69 76 70 90	209 210 234
31	3 9	55	159	73 107	229
32	6 7	58	160	74 76 77 79 110	217 230 232
33	5 6	60	161	65 72 84 85 87 110	204 209 230 233
34	4 13	54	162	66 85 89 111	209 234
35	6 9	58	163	73 110	219
36	6 9	58	164	70 83 90 94 96 97	204 212 232 235
37	6 11	63	165	79 83 89 91 93 109	209 212 231 232
38	5 12	56	166	64 84 89 102 122	216 218 219 234
39	7	58	167	68 84 97 125	216 230
40	7 11	61	168	69 84 85 98 112 125	218 230 233 234
41	8 12	61	169	70 85 101 124	219 233
42	8 12	87	170	71 72 92 98 117 120	218 228 233 241
43	11	55	171	72 99 118	210 230 241
44	7 10	62	172	73 80 117 118	229 237
45	8 14	60	173	74 81 86 91 94 111	214 215 226 232
46	9 12	80	174	75 76 89 99 100 120	210 215 217 242
47	10 12	60	175	75 81 83 92 104 121	214 215 218 242
48	11 12	58	176	76 76 94 101 123 124	213 232 246 242
49	12 13	62	177	77 86 96 98 115 120	211 228 232 239
50	11 14	62	178	77 87 92 101 107 116	214 220 233 239
51	12 14	63	179	78 90 94 95 105 106	217 219 224 235
52	14	98	180	78 102 103 113 114 115	220 227 231 234
53	15 18 21	129	181	83 103 108 121	213 231 240
54	18 19 20 22 33	129	182	94 97 105	214 221 235
55	17 24 30 41 42	135	183	82 93 97 105 106	205 213 243
56	27 38 39	135	184	86 87 99 112 118 126	216 217 226 230 234
57	20 33	129	185	103 104 110 122	215 225 240
58	28 31 35 41 48	129	186	89 102 113 119 121	216 224 227 232 236
59	26 38 51	133	187	51 102 103 109 113 121	212 225 226 231
60	32 36 44 46 47	131	188	92 98 99 118 126 127	213 230 236 241 242
61	39 40 48	130	189	93 100 104 118 124 125	212 215 227 242
62	43 48 49	130	190	95 101 105 109 114 116	214 219 223 224 243
63	37 50 52	145	191	96 101 112 116 120 123	205 212 233 239 243
64	46 41 52	131	192	97 106 109 112 115 120	217 221 225 232 243
65	15 18 19 20	129	193	88 98 125 92	211 218
66	16 22	133	194	107 110 117 123 124 125	205 220 225 229 233 236 238
67	17 18 17 28	133	195	107 118 123 127	212 229 238 239
68	18 24	135	196	108 111 119 122 125	213 215 222 125
69	18 19 23 35	133	197	110 118 125 127	213 229 238 240
70	19 27	134	198	114	223
71	15 23 43	137	199	115 116 123 126 168	214 224 225 139
72	15 24 29 41	133	200	117 118 127 128	226 227 237 238 241
73	16 41	139	201	119 121 126 127	222 224 226 240 242
74	17 20 26 28	134	202	120 126 127	221 222 227 230 241 242
75	17 21 24 31	133	203	129 132	0
76	23 43	138	204	120 130 133 134 137 138 140 141 156 161 164	245
77	20 23 27 40	140	205	130 131 143 144 147	245 246
78	22 26 27 32	134	206	134 135 143 144 147	246
79	22 28 37	145	207	136 141 143 148 149 154	247
80	16 45	145	208	150 151 152 153 155 156 157 158 160 161 162 165	248
81	17 29 30 46	142	209	172	249
82	32	129	210	132 145 158 171 174	253
83	32 33	129	211	147 152 171 183	251
84	10 29 34 49	137	212	145 146 147 149 164 165 189 191 195	250 251
85	19 34 38 49	138	213	130 142 150 174 176 181 189 195 197	249 250 252
86	20 29 35 48	138	214	140 141 145 173 176 182 190 194	245 247 251
87	20 24 38 41	135	215	136 139 142 153 174 175 185 189 195	247 252
88	21 23 29 48	133	216	135 128 142 153 166 167 184 186 187	248 249
89	22 36 38 42	135	217	140 141 145 172 173 176 184 192	247 251
90	22 35 37 43	139	218	137 137 140 153 166 168 170 175 193	246 253
91	26 30 33 36	135	219	134 138 144 150 166 169 173 179 190	245 248
92	23 24 41 48	139	220	139 143 147 150 160 178 184 194 196	247 250
93	25 30 35 37	139	221	149 152 162 192 202	247 251
94	26 33 42 47	141	222	153 154 196 201 202	247 252 253
95	27 32 33 39	141	223	144 151 187 190 198	246 248
96	27 31 40 43	140	224	147 149 151 192 199 196 190 190 201	247 248 251
97	32 33 35 40	140	225	146 146 150 153 185 187 192 194 191	246 247 250
98	29 50 51	146	226	142 143 149 155 173 184 187 200 201	247 248 250
99	24 29 45 51	142	227	148 148 154 154 180 189 250 252	247 250 253
100	25 31 45 50	145	228	156 157 170 177	255
101	27 38 44 47	144	229	159 163 172 194 195 197	254
102	30 38 46	143	230	157 161 167 188 171 184 188 199	250 255
103	30 46	142	231	165 180 181 187	249 250
104	31 41 46	142	232	160 164 165 173 176 177 186 192	250 251
105	32 39 40 43	136	233	156 161 168 169 170 178 191 194	245 255
106	32 37 40 46	150	234	158 162 166 168 176 180 186 196	249 253
107	41 47	146	235	164 179 182 183	245 251
108	42 100	146	236	194	246 254
109	33 37 38 48	138	237	172 200	247 254
110	41 49	130	238	194 195 137 200	250 254 255
111	42 50	139	239	177 178 184 188 191 195 199 202	250 251 255
112	35 38 50 51	148	240	181 185 202 197 201	249 250 251
113	36 37 46 48	150	241	170 171 188 200 202	253 255
114	47 49	151	242	174 175 176 188 189 193 201 202	251 252 253 254
115	47 49	152	243	183 190 191 192 244	243
116	47 47 48	146	244	196	252
117	41 51	145	245	204 205 214 218 219 233 234	0
118	41 51 52	142	246	205 223 225 236 243	0
119	42 46 51 51	142	247	207 208 214 215 217 220 221 222 224 225 226 227	256
120	43 48 50 51	145	248	206 208 216 217 221 224 226	0
121	46 51	151	249	209 213 213 230 231 231	251
122	46 49	150	250	212 213 229 228 226 227 231 232 238 239 240	256
123	47 51	137	251	211 212 214 217 221 224 232 235 236 242 243	256
124	47 49	151	252	213 215 225 244	252
125	40 51	153	253	210 218 222 227 234 241 242	0
126	48 50 51 52	148	254	229 236 237 238	257
127	51 52	140	255	228 230 233 238 239 241	0
128	52	152	256	247 250 251 252	0
			257	254	0

Our representation has the advantage, however, that it provides an easier visualization of the relationships between different polyhedra. Note that every convex polyhedron can be represented by a planar graph of connectivity at least three. Such a graph is obtained from our representation if the dotted edges are replaced by connexions drawn outside the basic polygon of order n , in such a way that they do not intersect. The completely triangulated polyhedra correspond to maximal planar graphs, *i.e.* they contain the maximum number of edges compatible with the non-intersection criterion.

There are two polyhedra of order five (Fig. 2). As described above, the second can be generated from the

first by the removal of an edge (or *vice-versa*); the arrow indicates this relationship.

There are seven polyhedra with six vertices, related as shown in Fig. 3; if the O_h octahedron were drawn in the more conventional form indicated as an alternative, then successive removal of inner edges to produce finally the trigonal prism (D_{3h}) is only possible if the order of vertices in the basic polygon is rearranged. Indeed, exhaustive removal of edges to leave the basic polygon without rearrangement of vertices is only possible for the polyhedra of order five and six; it is not possible for higher polyhedra in general.

The polyhedra with seven vertices are shown in Fig. 4. They are arranged first by the number of edges,

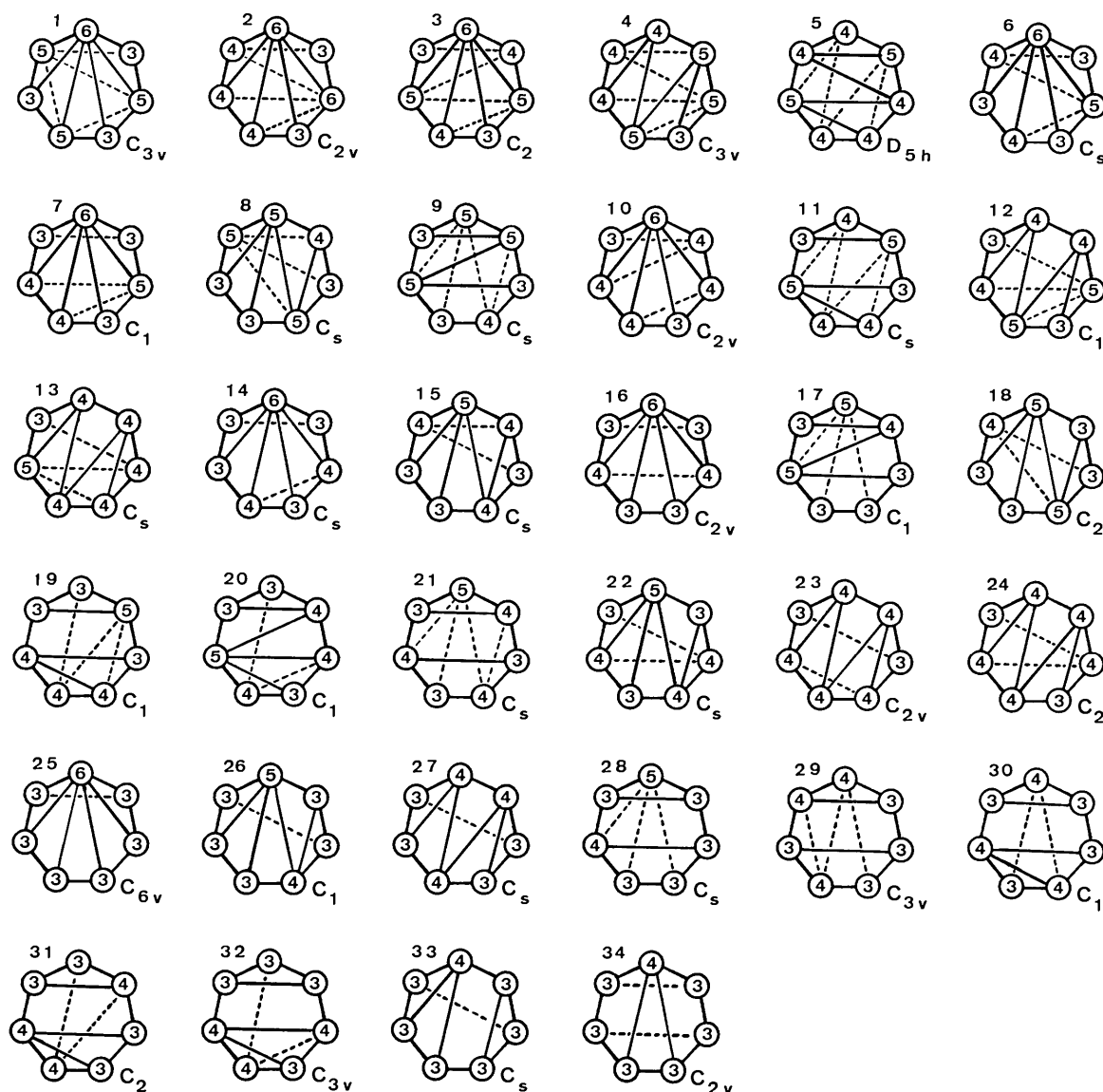


Fig. 4. The 34 polyhedra with seven vertices. The interrelationships are given in Table 1.

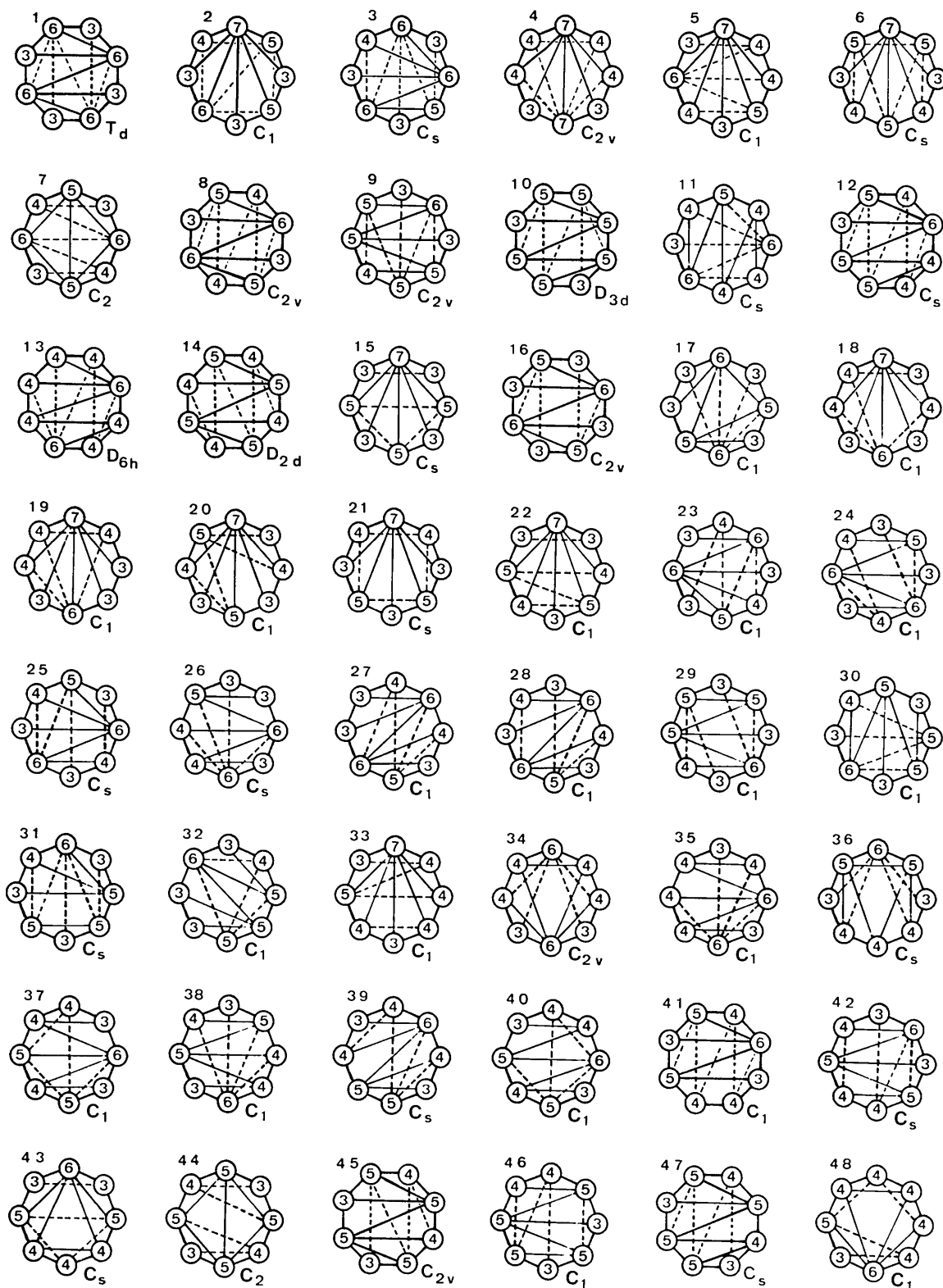


Fig. 5. The 257 polyhedra with eight vertices. The polyhedra related to the cube (No. 257) are distinguished by the different orientation of the octagon (*cf.* No. 256 and No. 257).

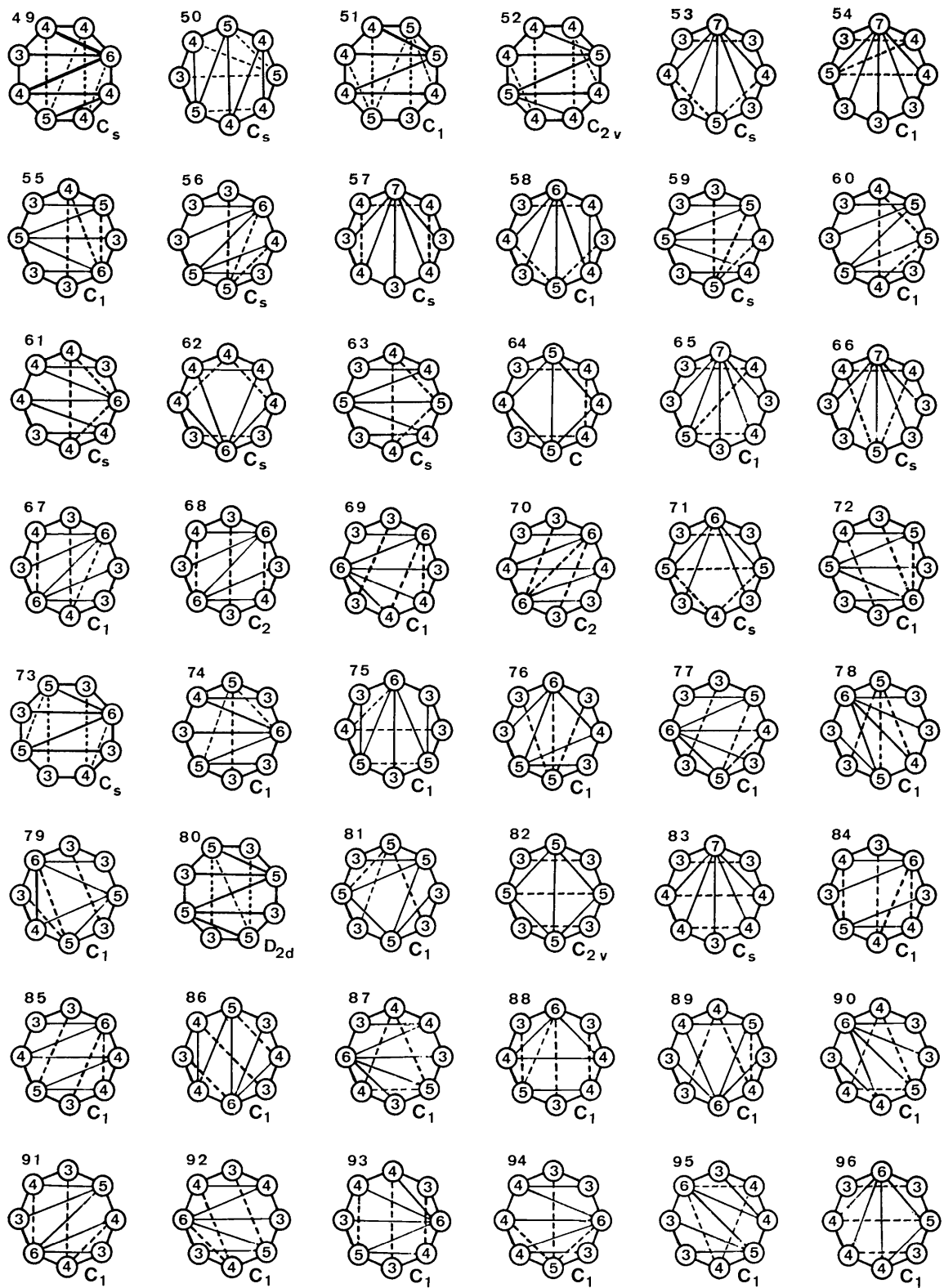


Fig. 5 (cont.)

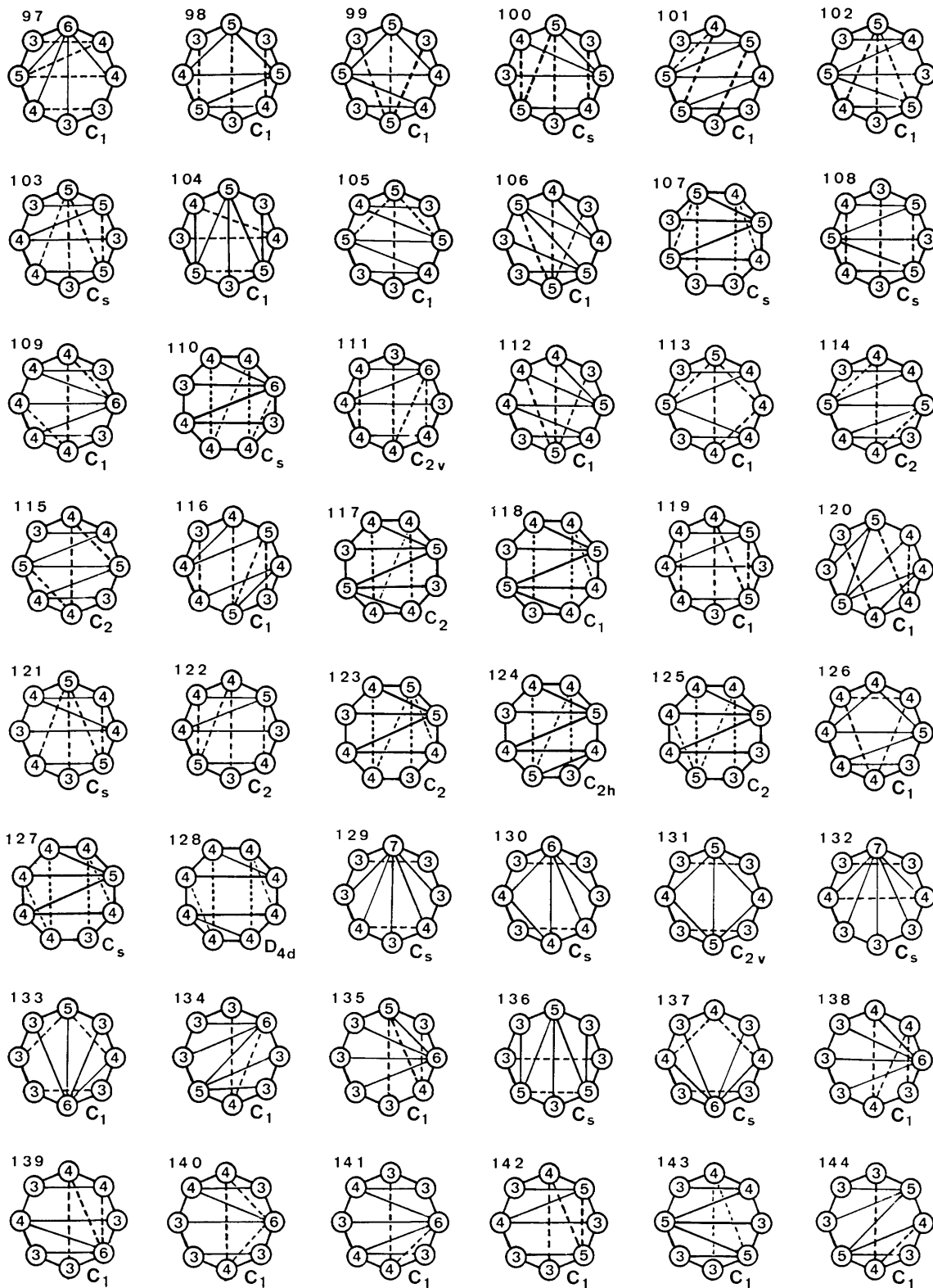


Fig. 5 (cont.)

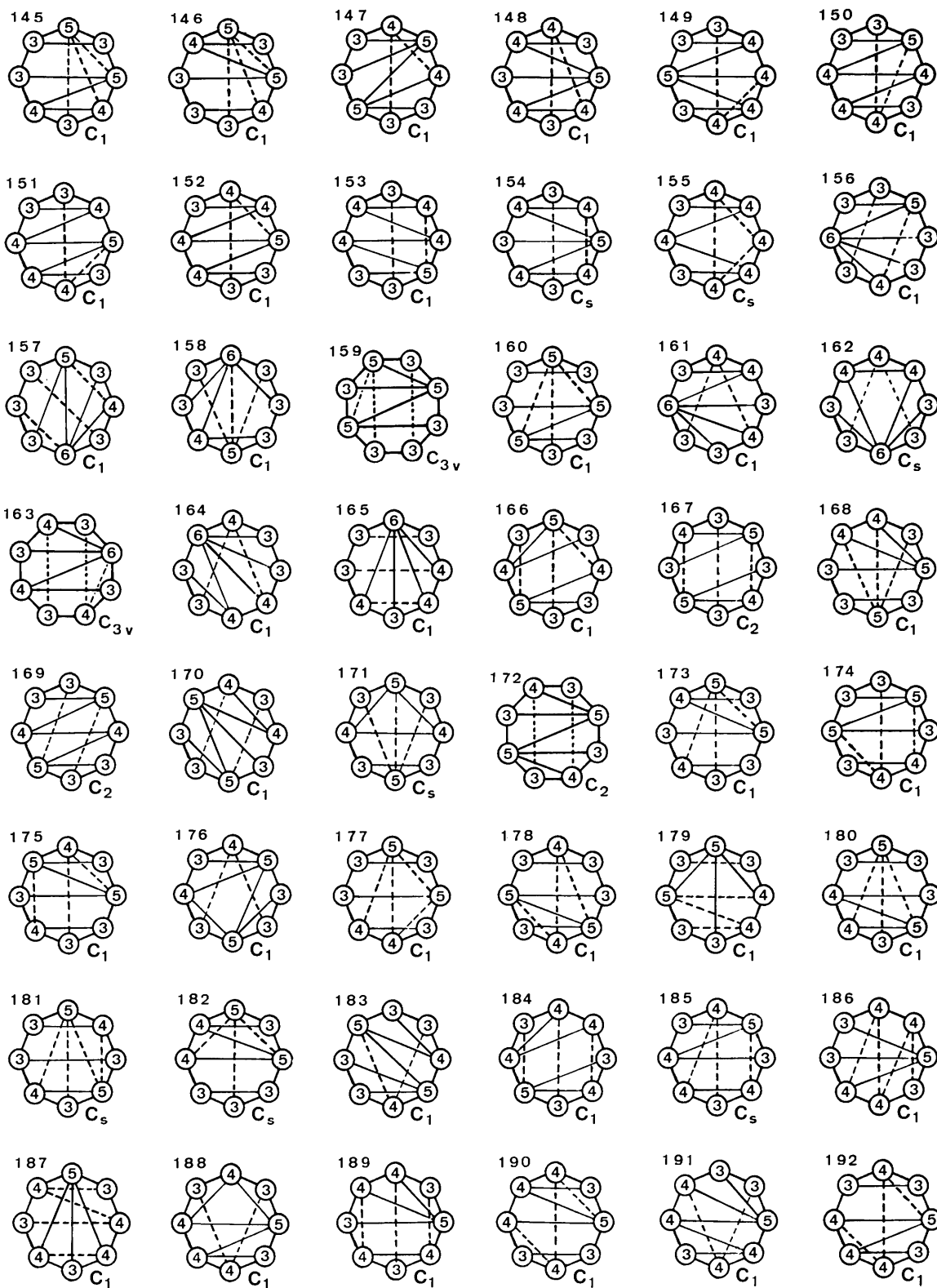


Fig. 5 (cont.)

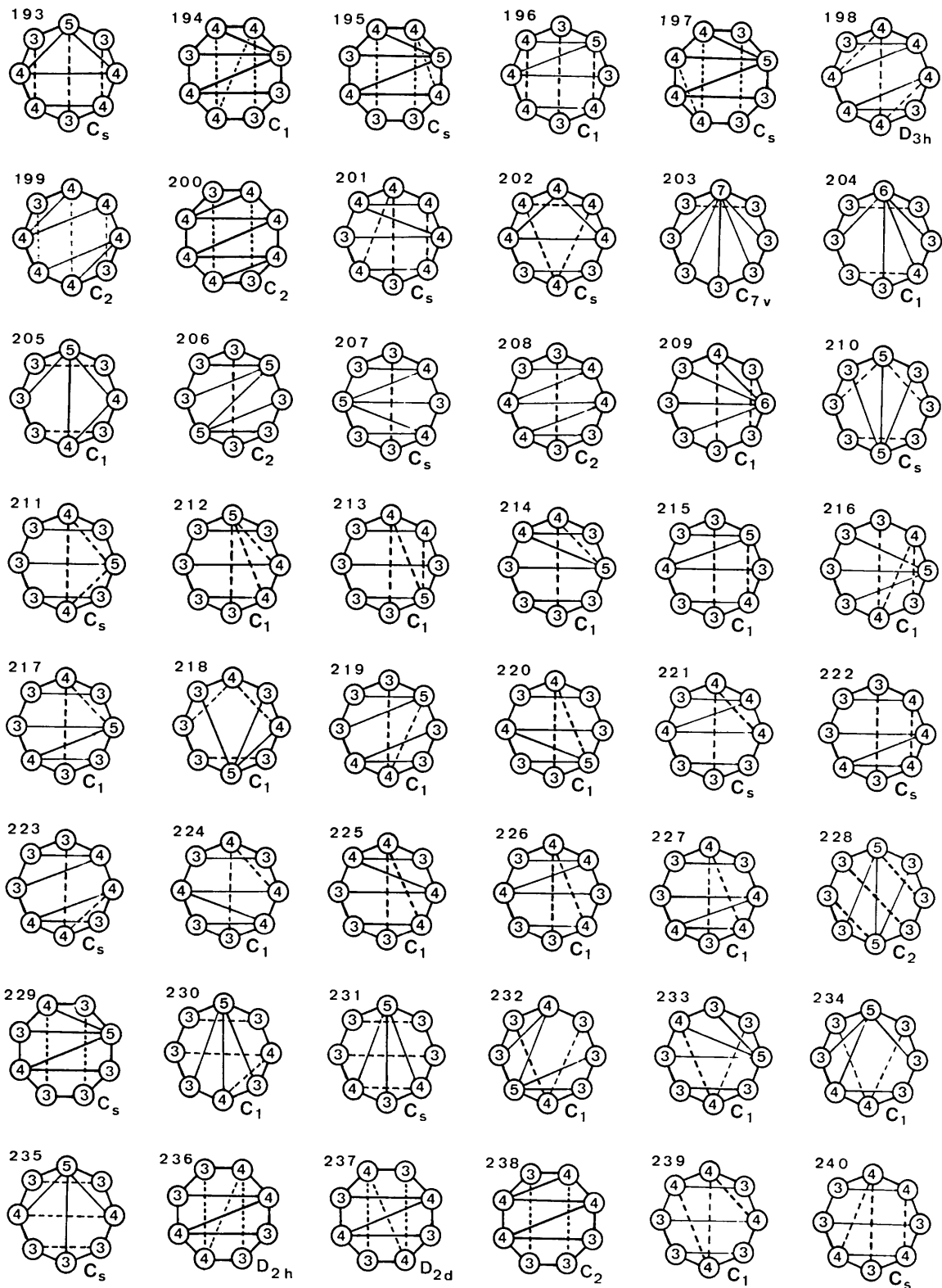


Fig. 5 (cont.)

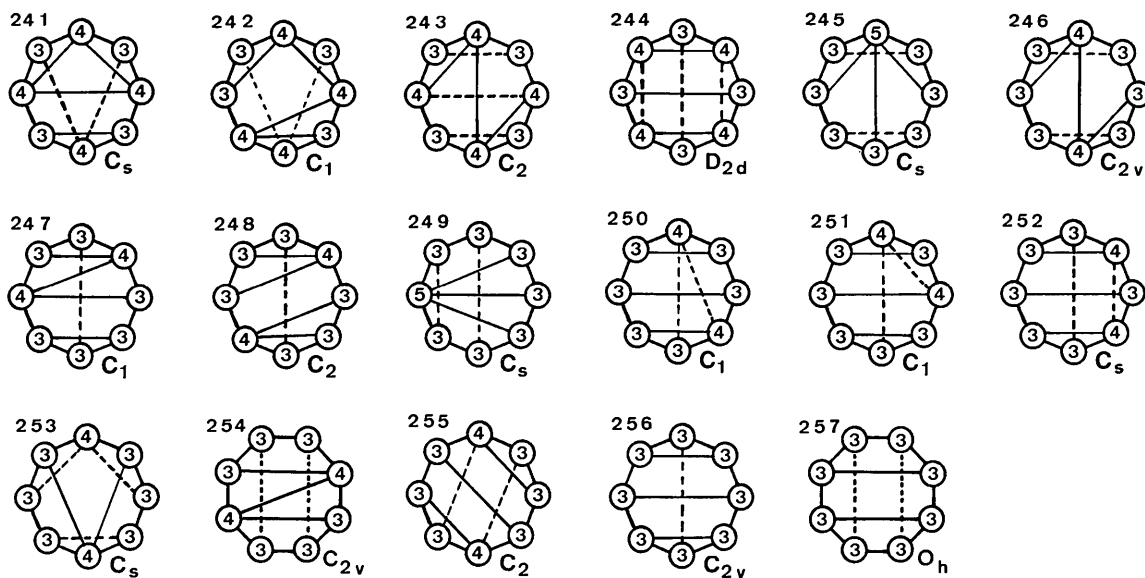


Fig. 5 (cont.)

then by the distribution of types of faces, then by the distribution of types of vertices, but this does not completely order the list, so they are also numbered arbitrarily from 1–34. Note, for example, that 17 and 18 are isomers in the sense that both have a face distribution $3_6 4_2 5_0 6_0$ and vertex distribution $3_4 4_1 5_2 6_0$ (in both codes the subscript indicates the number of faces or vertices with a given order). For polyhedra with seven vertices the inter-relationships are so complicated that a drawing (as provided in Fig. 3 for polyhedra with six vertices) would be more confusing than useful. These inter-relationships are described in Table 1.

The polyhedra with eight vertices are shown in Fig. 5. The 37 polyhedra that can be generated from the cube (No. 257) are shown with the basic octagon rotated by $\pi/8$ from the orientation used for the remain-

ing figures. The two other common coordination polyhedra with eight vertices, the Archimedean antiprism (No. 128), and the dodecahedron (No. 16), are also members of the family derived from the cube. The inter-relationships are given in Table 2.

This work was supported by the Swiss National Fund for the Advancement of Scientific Research. We thank Mrs L. aMarca and Miss H. Gächter for their help in drawing the figures.

References

- ALEXANDROW, A. D. (1958). *Convexe Polyeder*, p. 89. Berlin: Akademie-Verlag.
- GRACE, D. W. (1965). *Computer Search for Non-Isomorphic Convex Polyhedra*, Technical Report C515, Stanford University, Computer Science Department.