

the whole set of 00/ 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/ 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/	$c = +$	$c = -$	$c = +$	$c = -$	$c = +$	$c = -$	$c = +$	$c = -$
$l = 34$	+	+	+	+	-	-	-	-
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  $\Sigma_2$  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  $\Sigma_2$ . 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.

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## A Complete Catalogue of Polyhedra with Eight or Fewer Vertices

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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

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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

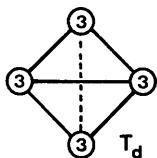


Fig. 1. The tetrahedron – the only polyhedron with four vertices.

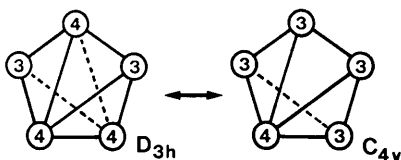


Fig. 2. The two polyhedra with five vertices.

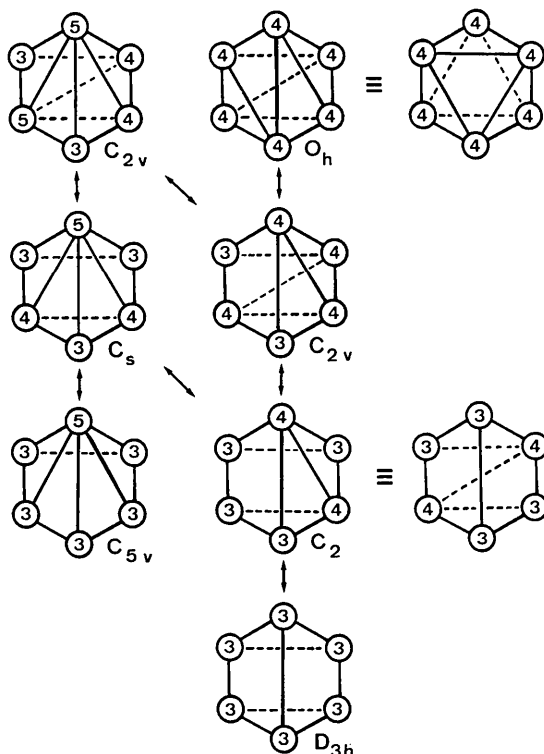


Fig. 3. The seven polyhedra with six vertices: these are shown in the left and centre columns. The right-hand column shows alternative representations for some of the polyhedra in the centre column. The arrows indicate relationship by the removal or addition of an edge.

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	.	.	.	.	.	.	.	.	.	19	22							
11	2	5	.	.	.	.	.	.	.	.	.	19	22							
12	3	4	.	.	.	.	.	.	.	.	15	17	19	20	20	24				
13	4	5	.	.	.	.	.	.	.	.	15	19	21	22	23	24				
14	6	7	10	.	.	.	.	.	.	.	.	25	26							
15	6	12	13	.	.	.	.	.	.	.	.	26	27							
16	7	.	.	.	.	.	.	.	.	.	.	28								
17	6	7	9	12	.	.	.	.	.	.	.	26	28	30						
18	7	8	.	.	.	.	.	.	.	.	.	26	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	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
26	14	15	17	18	19	20	22	.	.	.	.	.	.	.	.	.	.	.	.	.
27	15	20	23	24	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
28	16	17	19	21	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
29	21	23	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
30	17	19	21	22	23	24	.	.	.	.	.	.	.	.	.	.	.	.	.	.
31	18	19	20	24	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
32	20	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
33	26	27	30	31	32	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
34	28	29	30	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.

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

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,

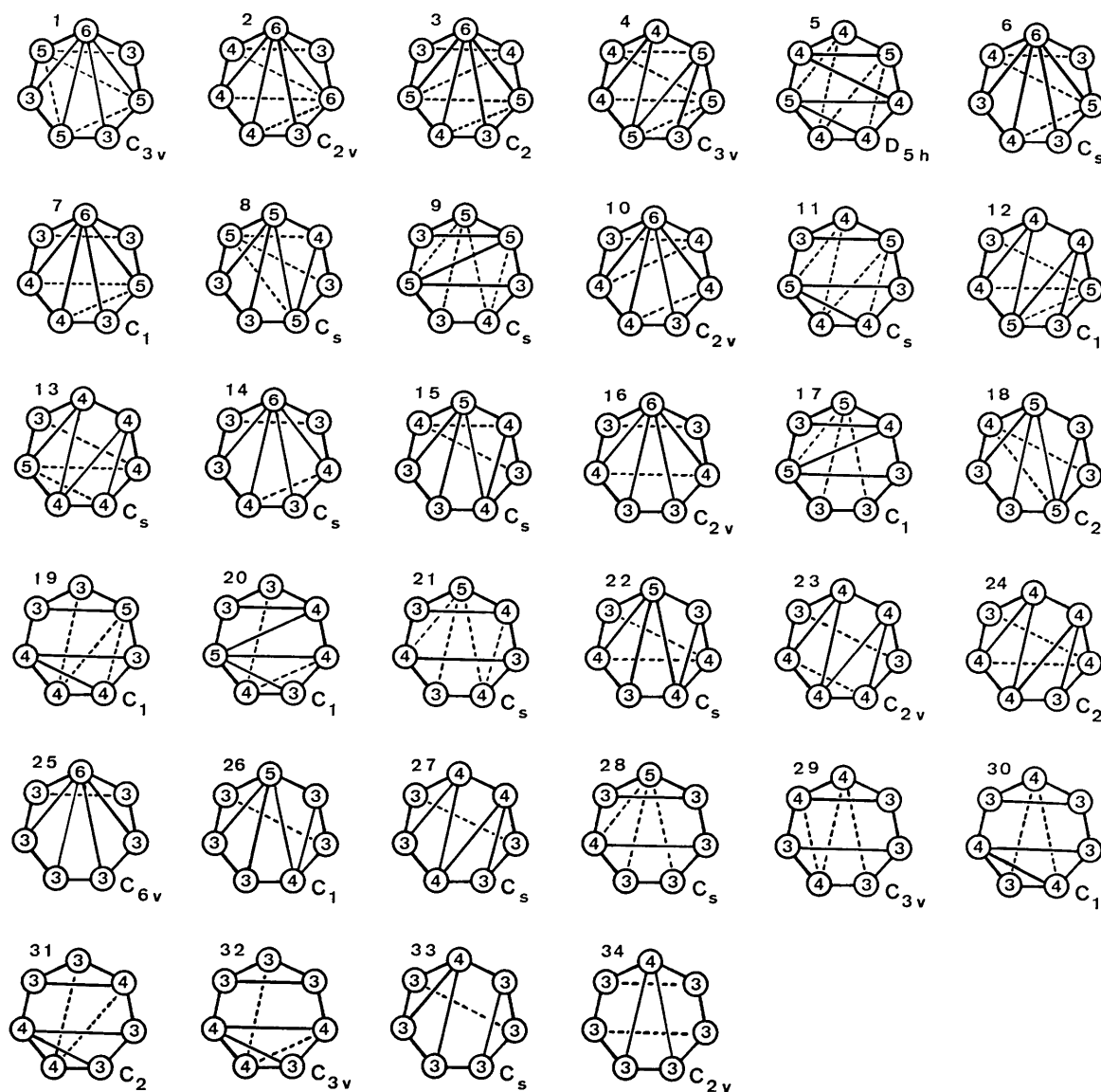


Fig. 4. The 34 polyhedra with seven vertices. The interrelationships are given in Table 1.

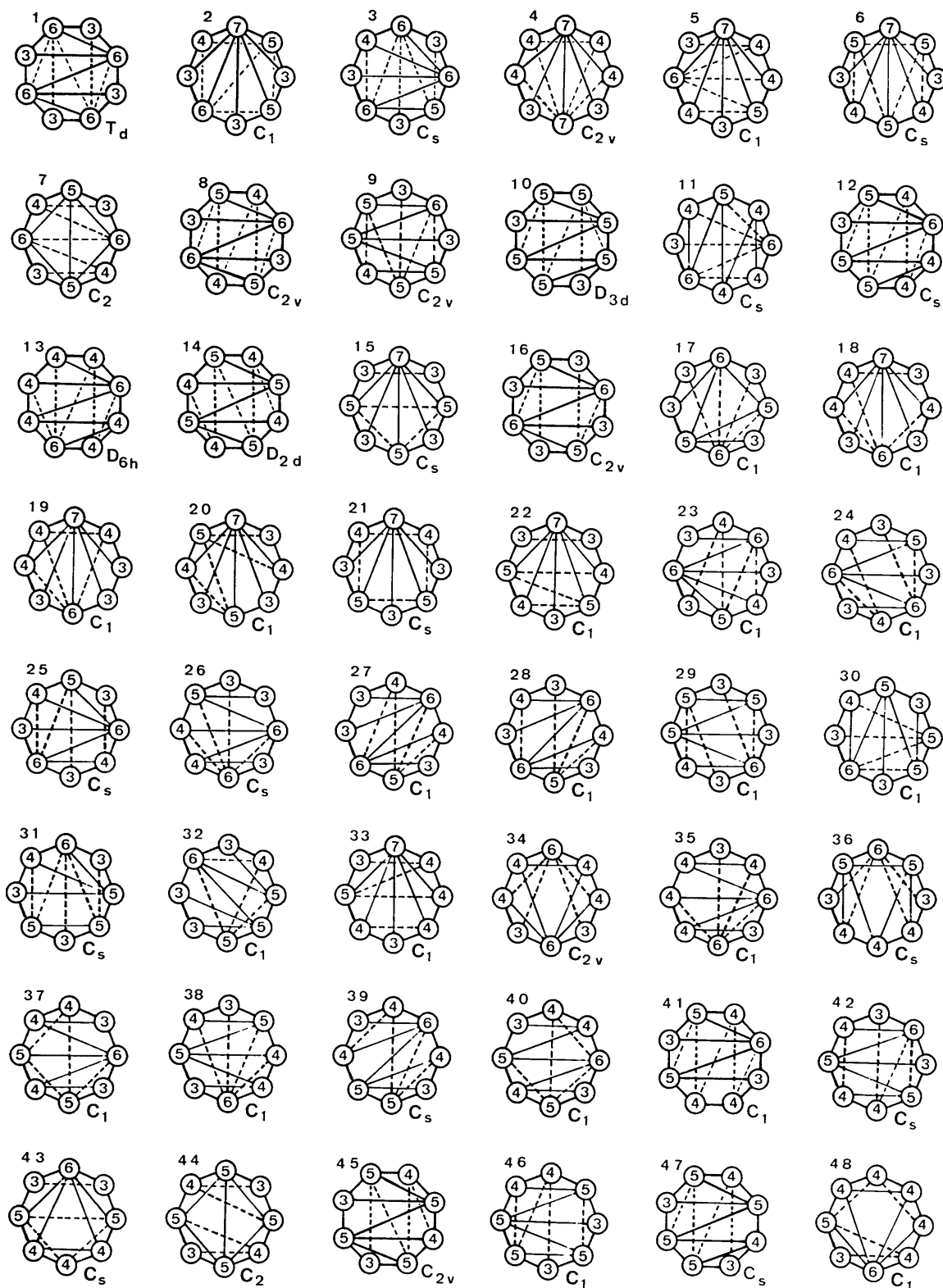


Fig. 5. The 257 polyhedra with eight vertices. The polyhedra related to the cube (No. 257) are distinguished by the different orientation of the octagon (*cf.* No. 256 and No. 257).

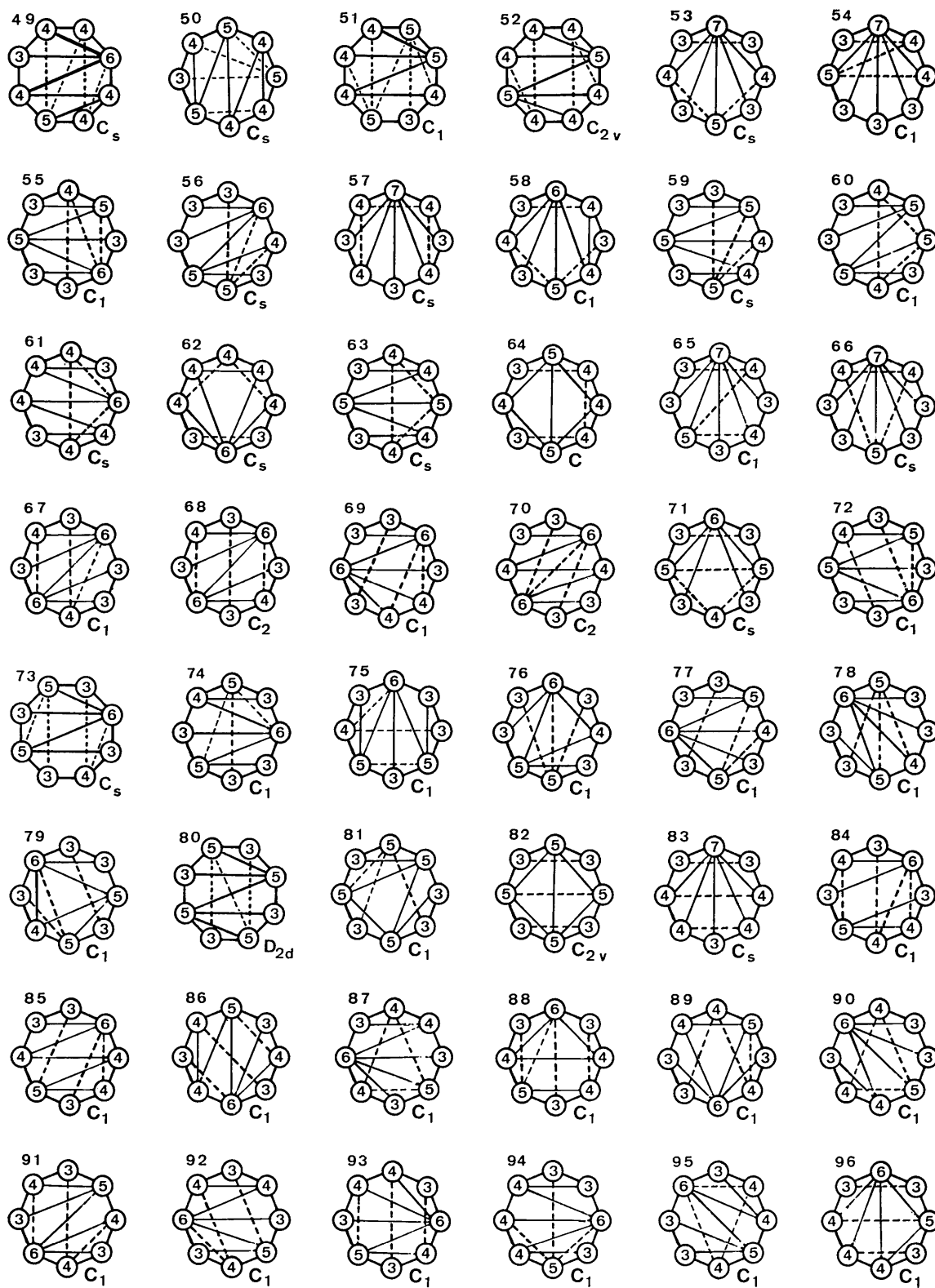


Fig. 5 (cont.)

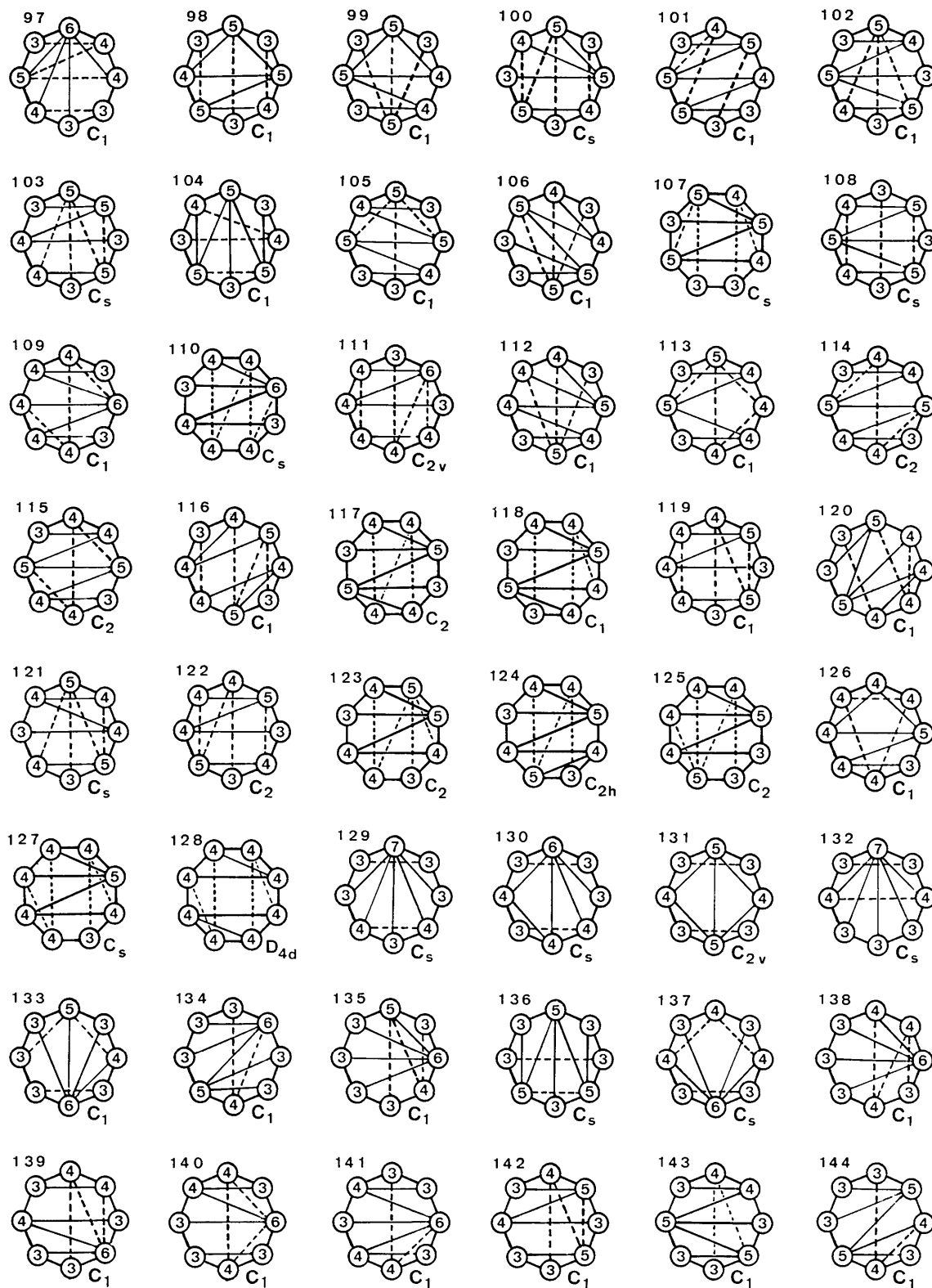


Fig. 5 (cont.)

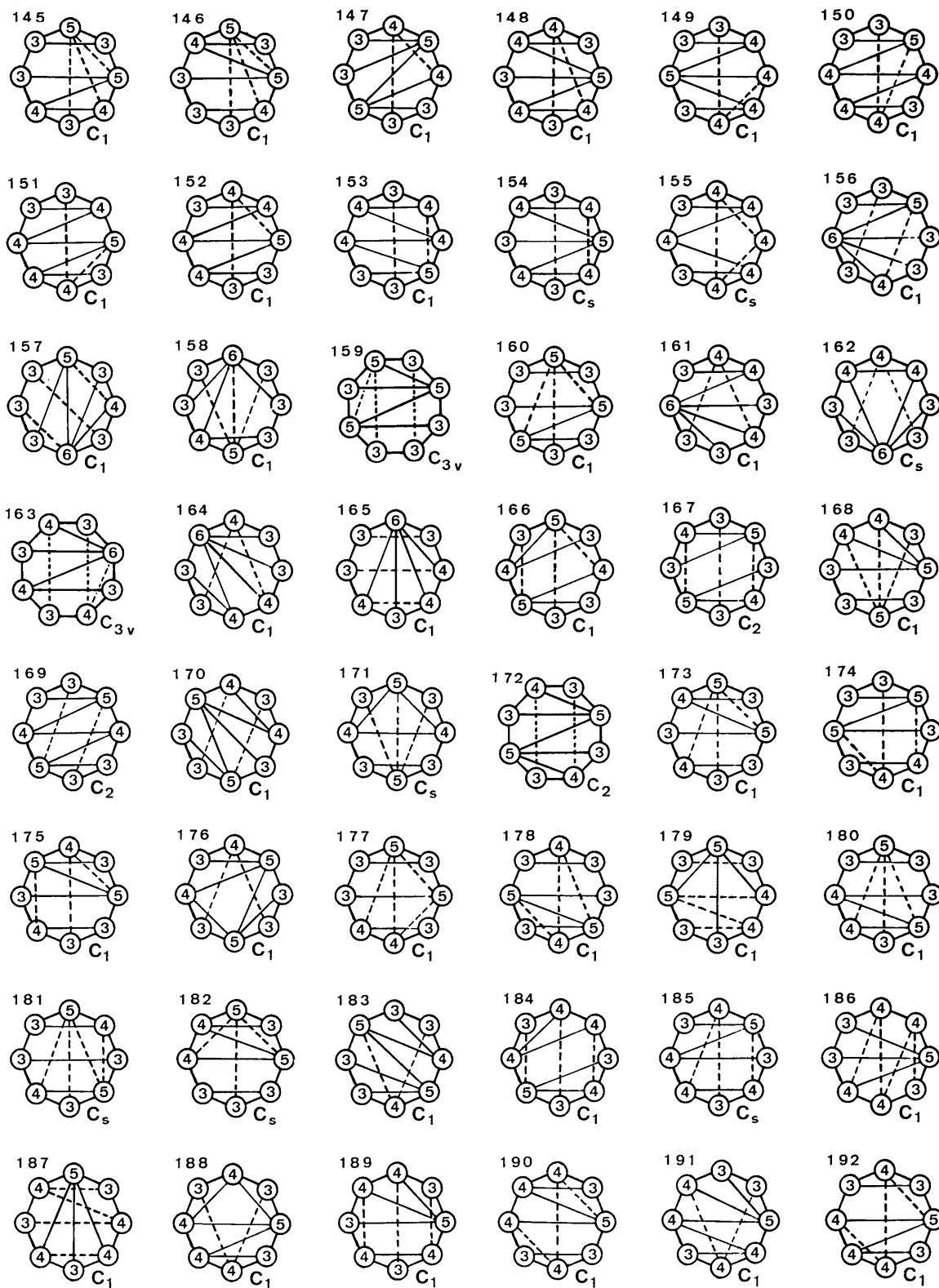


Fig. 5 (cont.)



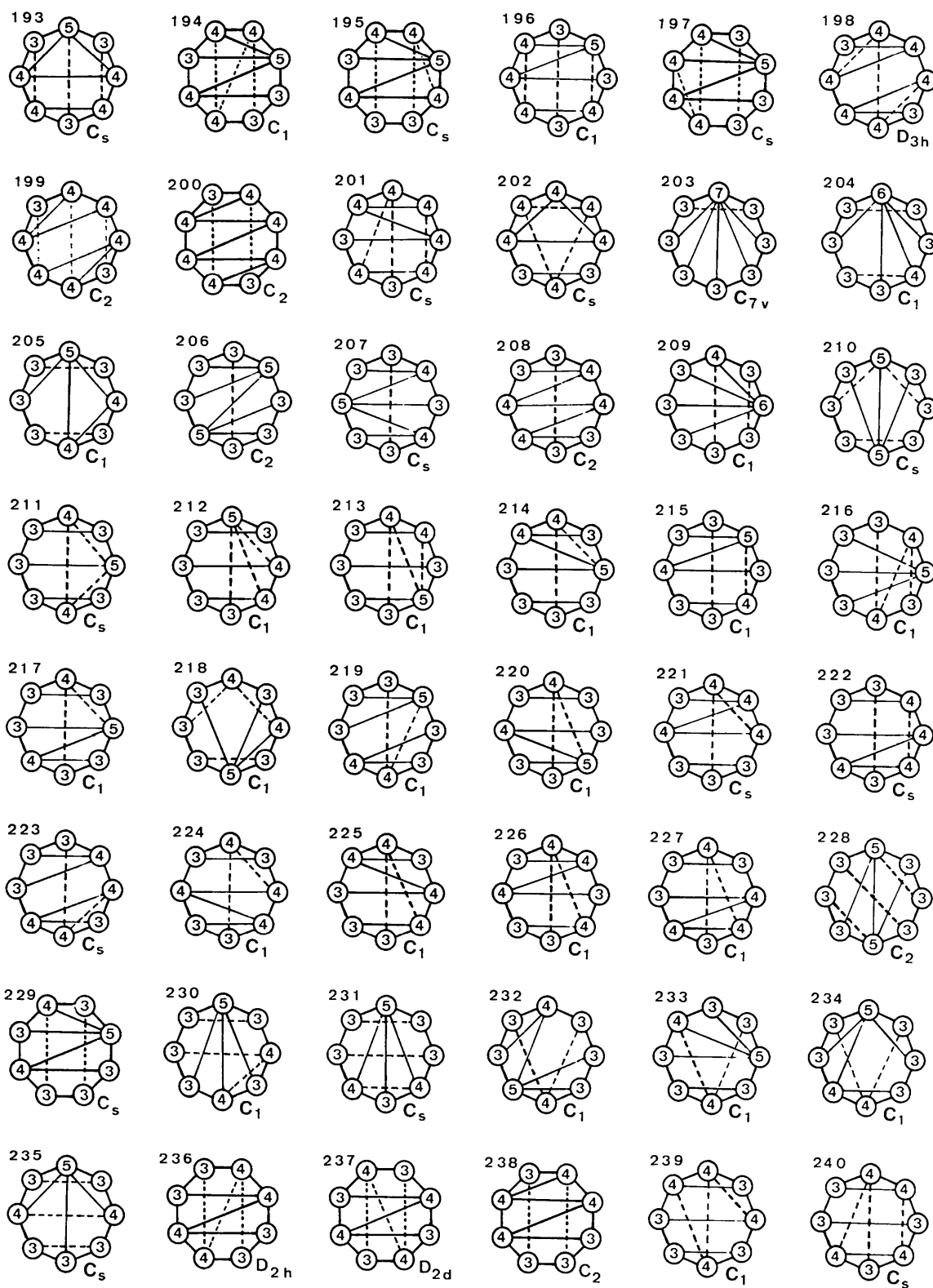


Fig. 5 (cont.)

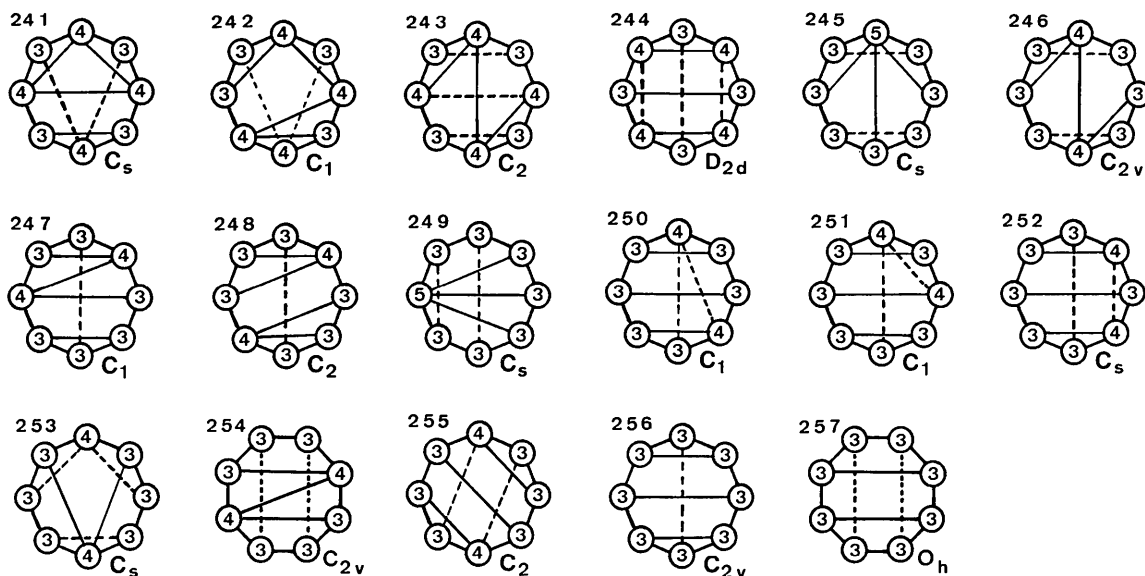


Fig. 5 (cont.)

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.

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