

Atomic environment classification of the rhombohedral “intermetallic” structure types

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Abstract

In this paper we give a complete description of the geometrical atomic environments found in the rhombohedral intermetallic structure types. Our analysis of 195 structure types showed that 144 are possible, while the remaining 51 structure types have *e.g.* improbable interatomic distances or are excluded because they are oxides with no intermetallic compounds crystallizing in this structure type.

In addition, we observed that 14 atomic environment types are greatly preferred. Out of 6356 investigated point sets, 4482 (71%) belong to one of these 14 atomic environment types. Of the 1324 compounds crystallizing in one of the 144 structure types, 19% belong to a single-environment group (structures in which all atoms have the same type of environment), 15% combine two environment types, 25% have three environments, 34% have four environments and the rest (7%) have five or more environments. Our systematic and comprehensive analysis of the rhombohedral structure types verified all known relationships between these structure types but also revealed new non-trivial relationships.

1. Introduction

In a previous paper [1], which can be regarded as the start of a complete and systematic continuation of the studies started in refs. 2 and 3, we have already discussed the importance of the crystal structure of a compound for its physical and/or chemical behaviour. It is therefore essential that the structures given in the literature should be correct or that they should be checked for their geometrical correctness, as we did for the cubic intermetallic structure types in ref. 1. In this investigation we report the results of our geometrical analysis of the 195 rhombohedral “intermetallic” structure types as they are compiled in ref. 4.

In ref. 1 we also pointed out the importance of atomic environments (AEs) for chemical crystallography and classified the cubic structure types on the basis of the observed atomic environments in these structure types.

In Table 1 the 195 structure types of the rhombohedral “intermetallic” compounds are arranged alphabetically according to the formula and in Table 2 according to the Pearson symbol. The structure type *hR16 Ga₇Rb* is in ref. 4 wrongly classified as belonging to the *hR16 Ga₃Pu* type, but in our analysis it is added to the list

because it is a different structure type. For the convenience of the reader the structure types have been numbered, so a structure of interest can easily be traced throughout the tables.

After analysing all 195 structure types, we excluded from our results all oxides (in so far as they did not have intermetallic compounds crystallizing in them, *e.g.* *hR19 O₁₂Pr₇*), all p-element structures or combinations between them, *e.g.* *hR2 O₂*, all structure types which are filled up with interstitial atoms such as hydrogen or nitrogen, *e.g.* *hR20 H₂HoNi₃*, and incompletely refined structure types, *e.g.* *hR7 Na₅Pb₂* in which the positions of the Na atoms were not refined in the publication. We also excluded the structure types consisting mainly of boron, *e.g.* *hR133 B₂₃Cu*, because these boron-rich structures can be regarded as structures consisting mainly of clusters of boron atoms, as will be shown later on.

In Tables 1 and 2 the excluded structure types are marked with an E in the last column where we normally give the number of atomic environments realized in the structure type. In practically all the excluded structure types we observed that, mainly owing to partly occupied point sets, improbable interatomic distances are realized, either too short or too long. In our geometrical analysis we can at this moment only analyse crystal structure descriptions with fully occupied point sets in so far as the partly occupied point sets do not

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TABLE 1. List of 195 rhombohedral "intermetallic" structure types ordered alphabetically; the structure type *hR16* Ga₇Rb was added to the list during printing. The structure types marked with an E in the last column were after the analysis (see text) excluded from our classification

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
1	<i>hR24</i>	AgAsS ₂	4	2
2	<i>hR14</i>	Ag ₃ AsS ₃	3	2
3	<i>hR15</i>	Ag ₂ Cr ₇ S ₁₂	6	E
4	<i>hR6</i>	AgCrSe ₂	4	2
5	<i>hR46</i>	Ag ₈ GeTe ₆	18	E
6	<i>hR42</i>	AgMg ₅ Zn ₉	15	2
7	<i>hR8</i>	AgNb ₄ S ₈	4	2
8	<i>hR8</i>	Ag ₈ Ta ₄	4	2
9	<i>hR44</i>	Al ₃ Au ₈	7	Poly
10	<i>hR137</i>	AlB ₃₁	19	E
11	<i>hR21</i>	AlB ₄₀ C ₄	5	E
12	<i>hR113</i>	AlB ₅₂ Cu	17	E
13	<i>hR7</i>	Al ₄ C ₃	4	3
14	<i>hR21</i>	Al ₆ C ₃ N ₂	11	E
15	<i>hR29</i>	Al ₈ C ₃ N ₄	15	E
16	<i>hR168</i>	AlCa ₃ Cd ₁₇	60	E
17	<i>hR26</i>	Al ₆ Cr ₅	9	2
18	<i>hR15</i>	Al ₃₁ Cu ₁₆ Ni ₄	8	Poly
19	<i>hR9</i>	Al ₄ Cu ₃ Zn	9	4
20	<i>hR20</i>	Al ₃ Ho	6	2
21	<i>hR10</i>	Al ₂ O ₃	2	2
22	<i>hR26</i>	AlPd	6	2
23	<i>hR14</i>	Al ₉ Sr ₅	6	Poly
24	<i>hR34</i>	Al ₇ Te ₁₀	8	3
25	<i>hR2</i>	As	1	1
26	<i>hR25</i>	As ₄ Cu ₆ Hg ₃ S ₁₂	9	2
27	<i>hR7</i>	As ₂ Cu ₄ Na	4	4
28	<i>hR26</i>	As ₆ Cu ₇ Se ₁₃	10	1
29	<i>hR17</i>	As ₅ Fe ₁₀ Ru ₂	9	Poly
30	<i>hR11</i>	As ₂ Ge ₇ Te ₆	6	2
31	<i>hR13</i>	As ₂ Ge ₄ Te ₇	7	2
32	<i>hR28</i>	As ₄ Pb ₉ S ₁₅	8	E
33	<i>hR7</i>	AsSe ₃ Tl ₃	3	3
34	<i>hR12</i>	AuNa ₃ S ₂	3	3
35	<i>hR13</i>	Au ₇ Rb ₄ Sn ₂	5	4
36	<i>hR6</i>	Au ₅ Sn	4	1
37	<i>hR12</i>	B	2	2
38	<i>hR111</i>	B	16	Poly
39	<i>hR141</i>	B	20	E
40	<i>hR105</i>	B	15	4
41	<i>hR31</i>	B ₁₂ Ba ₇ Ir ₁₂	6	Poly
42	<i>hR34</i>	B ₆ Ba ₂ Ni ₉	4	3
43	<i>hR15</i>	B ₁₃ C ₂	4	3
44	<i>hR29</i>	B ₁₉ C	6	E
45	<i>hR12</i>	B ₂ CU	4	4
46	<i>hR96</i>	B ₈ Ce ₁₅ N ₂₅	10	E
47	<i>hR13</i>	B ₆ Co ₂ Pr ₅	5	3
48	<i>hR13</i>	B ₆ Co ₃ Tb ₄	5	4
49	<i>hR18</i>	B ₂ Co ₃ Zr	5	4
50	<i>hR133</i>	B ₂₃ Cu	20	E
51	<i>hR133</i>	B ₂₈ Cu	20	E
52	<i>hR113</i>	B ₄₉ Fe	17	E
53	<i>hR12</i>	B ₃ FeNd ₂	4	E
54	<i>hR155</i>	B ₉₀ Ge	22	E
55	<i>hR10</i>	B ₄ Li ₅	4	E

(continued)

TABLE 1. (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
56	<i>hR115</i>	B ₂₃ Mn	18	E
57	<i>hR7</i>	B ₅ Mo ₂	4	4
58	<i>hR143</i>	B ₉₇ Ni ₂	20	E
59	<i>hR19</i>	B ₆ Ni ₁₂ Sr	4	4
60	<i>hR14</i>	B ₆ P	3	2
61	<i>hR119</i>	B ₂₈ Sc	18	E
62	<i>hR121</i>	B ₂₅ Zn	19	E
63	<i>hR119</i>	B ₅₁ Zr	18	E
64	<i>hR31</i>	Ba ₂ NbS ₅	8	E
65	<i>hR12</i>	BaPb ₃	4	2
66	<i>hR12</i>	Be ₃ Nb	5	3
67	<i>hR19</i>	Be ₁₇ Nb ₂	5	4
68	<i>hR11</i>	Bi ₂ Ge ₃ Te ₆	11	1
69	<i>hR16</i>	BiMn ₃	4	3
70	<i>hR2</i>	BiO	2	E
71	<i>hR7</i>	Bi ₃ Se ₄	4	1
72	<i>hR17</i>	Bi ₈ Se ₉	9	1
73	<i>hR5</i>	Bi ₇ Te ₃	3	1
74	<i>hR44</i>	C ₄ HgN ₄ Rb ₂	7	E
75	<i>hR22</i>	C ₂ Mn ₁₇ Pr ₂	6	E
76	<i>hR8</i>	CNi ₃	2	2
77	<i>hR16</i>	CSi	16	4
78	<i>hR62</i>	CSi	62	E
79	<i>hR13</i>	C ₅ Ti ₈	5	3
80	<i>hR6</i>	CaSi ₂	3	3
81	<i>hR24</i>	Ce ₅ Co ₁₉	9	Poly
82	<i>hR15</i>	CeMo ₆ S ₈	4	4
83	<i>hR21</i>	Ce ₇ O ₁₂	5	E
84	<i>hR53</i>	Co ₅ Cr ₂ Mo ₃	11	4
85	<i>hR18</i>	Co ₇ Er ₂	7	3
86	<i>hR20</i>	Co ₄ Fe ₄ Th	6	E
87	<i>hR32</i>	Co ₂ Ge ₃ S ₃	12	2
88	<i>hR5</i>	CrCuS ₂	5	E
89	<i>hR4</i>	CrCuSe ₂	4	4
90	<i>hR4</i>	CrNaS ₂	3	1
91	<i>hR9</i>	Cr ₇ Na ₂ Se ₁₂	5	3
92	<i>hR10</i>	Cr ₂ S ₃	4	4
93	<i>hR28</i>	CsMo ₆ Se ₇	6	Poly
94	<i>hR14</i>	Cu ₅ FeS ₄	8	E
95	<i>hR4</i>	Cu ₂ GaSr	3	3
96	<i>hR26</i>	Cu ₇ Hg ₆	9	Poly
97	<i>hR8</i>	Cu ₃ K ₃ P ₂	4	4
98	<i>hR13</i>	CuMo ₃ S ₄	5	E
99	<i>hR6</i>	Cu ₃ NaTe ₂	6	Poly
100	<i>hR9</i>	CuNb ₆ S ₁₀	5	3
101	<i>hR17</i>	Cu ₂ P ₂ Yb	9	Poly
102	<i>hR12</i>	Cu ₅ P ₄ Yb ₂	6	4
103	<i>hR26</i>	Cu ₉ S ₅	14	E
104	<i>hR15</i>	Er ₃ Ni ₂	4	3
105	<i>hR38</i>	Eu ₂ Re ₆ S ₁₁	5	4
106	<i>hR9</i>	Fe ₂ Ga ₂ S ₅	5	3
107	<i>hR21</i>	FeMo ₁₂ S ₁₆ Sn ₂	5	Poly
108	<i>hR10</i>	FePSe ₃ -a	3	3
109	<i>hR10</i>	FePSe ₃ -b	6	3
110	<i>hR7</i>	Fe ₃ S ₄	4	4
111	<i>hR10</i>	Fe ₃ Sn ₂	3	3
112	<i>hR6</i>	Fe ₂ Tb	3	2
113	<i>hR13</i>	Fe ₇ W ₆	5	4
114	<i>hR22</i>	Ga	5	4

(continued)

TABLE 1. (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
115	<i>hR138</i>	Ga ₅₀ K ₄ Na ₁₃	20	Poly
116	<i>hR5</i>	Ga ₂ Li ₃	3	1
117	<i>hR20</i>	Ga ₁₄ Li ₃	4	3
118	<i>hR120</i>	Ga ₁₃ Na ₇	18	Poly
119	<i>hR14</i>	Ga ₄ Pd ₇ Zn ₃	6	2
120	<i>hR16</i>	Ga ₃ Pu	4	2
121	<i>hR4</i>	GaSe	4	2
122	<i>hR49</i>	Ga ₄₁ V ₈	11	Poly
123	<i>hR38</i>	Ge ₃ La ₄ S ₁₂	7	4
124	<i>hR6</i>	GeRh ₃ Y ₂	3	2
125	<i>hR2</i>	GeTe	9	E
126	<i>hR20</i>	H ₂ HoNi ₃	7	E
127	<i>hR14</i>	H ₄ N ₂ Th	3	E
128	<i>hR23</i>	HP ₄ Pd ₃₀	6	E
129	<i>hR1</i>	Hg	1	1
130	<i>hR2</i>	HgIn	2	1
131	<i>hR24</i>	HgMg ₃	7	4
132	<i>hR16</i>	InMg ₃	8	E
133	<i>hR72</i>	In ₂ Mo ₁₅ Se ₁₉	9	Poly
134	<i>hR73</i>	In ₄ SSe ₂ Te ₃	15	E
135	<i>hR7</i>	In ₂ S ₄ Zn	7	3
136	<i>hR14</i>	In ₂ S ₄ Zn	14	3
137	<i>hR9</i>	In ₂ S ₅ Zn ₂	9	3
138	<i>hR5</i>	In ₂ Se ₃	5	3
139	<i>hR44</i>	In ₃ Yb ₈	7	Poly
140	<i>hR12</i>	Ir ₃ Se ₈	4	2
141	<i>hR16</i>	K ₃ SbSe ₄	4	3
142	<i>hR26</i>	Li ₃ Mo ₉ S ₁₂	5	E
143	<i>hR10</i>	Li ₅ NaSn ₄	10	4
144	<i>hR22</i>	Li ₅ Na ₂ Sn ₄	11	4
145	<i>hR7</i>	Li ₇ Si ₃	4	1
146	<i>hR26</i>	Mo ₃ NiS ₄	5	E
147	<i>hR15</i>	Mo ₈ PbS ₈	4	4
148	<i>hR42</i>	Mo ₉ Rb ₂ Se ₁₀	9	Poly
149	<i>hR3</i>	MoS ₂	3	2
150	<i>hR17</i>	Mo ₈ S ₈ Sn	5	E
151	<i>hR44</i>	Mo ₉ S ₁₁ Tl ₂	10	4
152	<i>hR14</i>	Mo ₃ Se ₄	3	3
153	<i>hR16</i>	N	2	E
154	<i>hR3</i>	N ₂ W	2	2
155	<i>hR5</i>	N ₆ W ₇	3	3
156	<i>hR7</i>	Na ₅ Pb ₂	1	E
157	<i>hR8</i>	Na ₂ S ₂ Sn	3	E
158	<i>hR4</i>	NaS ₄ Ti ₂	4	3
159	<i>hR4</i>	NbS ₂	4	2
160	<i>hR7</i>	Ni ₃ Pb ₂ S ₂	4	4
161	<i>hR6</i>	NiS	2	2
162	<i>hR5</i>	Ni ₃ S ₂	2	2
163	<i>hR7</i>	Ni ₃ S ₂ Sn ₂	4	4
164	<i>hR5</i>	Ni ₃ Se ₂	2	2
165	<i>hR4</i>	NiTe	2	2
166	<i>hR7</i>	Ni ₂ Ti	4	2
167	<i>hR2</i>	O ₂	1	E
168	<i>hR28</i>	O ₃ P ₂	6	E
169	<i>hR19</i>	O ₁₂ Pr ₇	4	E
170	<i>hR16</i>	OZr ₃	5	E
171	<i>hR17</i>	P ₂ Pd ₁₅	5	4
172	<i>hR20</i>	P ₃ Pd ₇	8	Poly
173	<i>hR38</i>	P ₁₃ Re ₆	7	3

(continued)

TABLE 1. (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
174	<i>hR32</i>	P ₁₆ Si ₉ Sn ₄	12	4
175	<i>hR8</i>	P ₃ Sn	2	2
176	<i>hR14</i>	Pd ₄ Pu ₃	4	3
177	<i>hR44</i>	Pd ₈ Sb ₃ -a	12	Poly
178	<i>hR44</i>	Pd ₈ Sb ₃ -b	24	Poly
179	<i>hR27</i>	Pd ₂₀ Sb ₇	6	3
180	<i>hR92</i>	Re ₂₅ Zr ₂₁	10	3
181	<i>hR22</i>	Rh ₃ ScSi ₇	4	4
182	<i>hR11</i>	Rh ₃ Se ₈	3	3
183	<i>hR6</i>	S ₂ Ta	6	3
184	<i>hR6</i>	STi	4	2
185	<i>hR14</i>	S ₄ Ti ₃	8	2
186	<i>hR22</i>	S ₁₁ Ti ₈	12	2
187	<i>hR8</i>	S ₁₂ Ti ₇	5	2
188	<i>hR14</i>	S ₁₄ Ti ₁₁	8	2
189	<i>hR27</i>	STl ₂	9	E
190	<i>hR22</i>	Sb ₃ Zn ₄	3	3
191	<i>hR6</i>	Se	1	1
192	<i>hR8</i>	Se ₄ Zr ₃	4	1
193	<i>hR3</i>	Sm	2	2
194	<i>hR19</i>	Th ₂ Zn ₁₇	5	4
195	<i>hR16</i>	Ga ₇ Rb	4	4

E, excluded.

TABLE 2. List of 195 rhombohedral "intermetallic" structure types ordered according to Pearson symbol; the structure type *hR16* Ga₇Rb was added to the list during printing. The structure types marked with an E in the last column were after the analysis (see text) excluded from our classification

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
129	<i>hR1</i>	Hg	1	1
25	<i>hR2</i>	As	1	1
70	<i>hR2</i>	BiO	2	E
125	<i>hR2</i>	GeTe	2	E
130	<i>hR2</i>	HgIn	2	1
167	<i>hR2</i>	O ₂	1	E
149	<i>hR3</i>	MoS ₂	3	2
154	<i>hR3</i>	N ₂ W	2	2
193	<i>hR3</i>	Sm	2	2
89	<i>hR4</i>	CrCuSe ₂	4	4
90	<i>hR4</i>	CrNaS ₂	3	1
95	<i>hR4</i>	Cu ₂ GaSr	3	3
121	<i>hR4</i>	GaSe	4	2
158	<i>hR4</i>	NaS ₄ Ti ₂	4	3
159	<i>hR4</i>	NbS ₂	4	2
165	<i>hR4</i>	NiTe	2	2
73	<i>hR5</i>	Bi ₂ Te ₃	3	1
88	<i>hR5</i>	CrCuS ₂	5	E
116	<i>hR5</i>	Ga ₂ Li ₃	3	1
138	<i>hR5</i>	In ₂ Se ₃	5	3
155	<i>hR5</i>	N ₆ W ₇	3	3
162	<i>hR5</i>	Ni ₃ S ₂	2	2
164	<i>hR5</i>	Ni ₃ Se ₂	2	2

(continued)

TABLE 2. (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
4	<i>hR6</i>	AgCrSe ₂	4	2
36	<i>hR6</i>	Au ₅ Sn	4	1
80	<i>hR6</i>	CaSi ₂	3	3
99	<i>hR6</i>	Cu ₃ NaTe ₂	6	Poly
112	<i>hR6</i>	Fe ₂ Tb	3	2
124	<i>hR6</i>	GeRh ₃ Y ₂	3	2
161	<i>hR6</i>	NiS	2	2
183	<i>hR6</i>	S ₂ Ta	6	3
184	<i>hR6</i>	STi	4	2
191	<i>hR6</i>	Se	1	1
13	<i>hR7</i>	Al ₄ C ₃	4	3
27	<i>hR7</i>	As ₂ Cu ₄ Na	4	4
33	<i>hR7</i>	AsSe ₃ Tl ₃	3	3
57	<i>hR7</i>	B ₅ Mo ₂	4	4
71	<i>hR7</i>	Bi ₃ Se ₄	4	1
110	<i>hR7</i>	Fe ₃ S ₄	4	4
135	<i>hR7</i>	In ₂ S ₄ Zn	7	3
145	<i>hR7</i>	Li ₇ Si ₃	4	1
156	<i>hR7</i>	Na ₅ Pb ₂	1	E
160	<i>hR7</i>	Ni ₃ Pb ₂ S ₂	4	4
163	<i>hR7</i>	Ni ₃ S ₂ Sn ₂	4	4
166	<i>hR7</i>	Ni ₂ Ti	4	2
7	<i>hR8</i>	AgNb ₄ S ₈	4	2
8	<i>hR8</i>	AgS ₈ Ta ₄	4	2
76	<i>hR8</i>	CNi ₃	2	2
97	<i>hR8</i>	Cu ₃ K ₃ P ₂	4	4
157	<i>hR8</i>	Na ₂ S ₃ Sn	3	E
175	<i>hR8</i>	P ₃ Sn	2	2
187	<i>hR8</i>	S ₁₂ Ti ₇	5	2
192	<i>hR8</i>	Se ₄ Zr ₃	4	1
19	<i>hR9</i>	Al ₄ Cu ₃ Zn	9	4
91	<i>hR9</i>	Cr ₇ Na ₂ Se ₁₂	5	3
100	<i>hR9</i>	CuNb ₆ S ₁₀	5	3
106	<i>hR9</i>	Fe ₂ Ga ₂ S ₅	5	3
137	<i>hR9</i>	In ₂ S ₅ Zn ₂	9	2
21	<i>hR10</i>	Al ₂ O ₃	2	2
55	<i>hR10</i>	B ₄ Li ₅	4	E
92	<i>hR10</i>	Cr ₂ S ₃	4	4
108	<i>hR10</i>	FePSe ₃ - a	3	3
109	<i>hR10</i>	FePSe ₃ - b	6	3
111	<i>hR10</i>	Fe ₃ Sn ₂	3	3
143	<i>hR10</i>	Li ₅ NaSn ₄	10	4
30	<i>hR11</i>	As ₂ Ge ₃ Te ₆	6	2
68	<i>hR11</i>	Bi ₂ Ge ₃ Te ₆	11	1
182	<i>hR11</i>	Rh ₃ Se ₈	3	3
34	<i>hR12</i>	AuNa ₃ S ₂	3	3
37	<i>hR12</i>	B	2	2
45	<i>hR12</i>	B ₂ Cu	4	4
53	<i>hR12</i>	B ₃ FeNd ₂	4	E
65	<i>hR12</i>	BaPb ₃	4	2
66	<i>hR12</i>	Be ₃ Nb	5	3
102	<i>hR12</i>	Cu ₅ P ₄ Yb ₂	6	4
140	<i>hR12</i>	Ir ₃ Se ₈	4	2
31	<i>hR13</i>	As ₂ Ge ₄ Te ₇	7	2
35	<i>hR13</i>	Au ₇ Rb ₄ Sn ₂	5	4
47	<i>hR13</i>	B ₆ Co ₂ Pr ₅	5	3
48	<i>hR13</i>	B ₆ Co ₃ Tb ₄	5	4
79	<i>hR13</i>	C ₅ Ti ₈	5	3
98	<i>hR13</i>	CuMo ₃ S ₄	5	E

(continued)

TABLE 2 (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
113	<i>hR13</i>	Fe ₇ W ₆	5	4
2	<i>hR14</i>	Ag ₃ AsS ₃	3	2
23	<i>hR14</i>	Al ₅ Sr ₅	6	Poly
60	<i>hR14</i>	B ₆ P	3	2
94	<i>hR14</i>	Cu ₅ FeS ₄	8	E
119	<i>hR14</i>	Ga ₄ Pd ₇ Zn ₃	6	2
127	<i>hR14</i>	H ₄ N ₂ Th	3	E
136	<i>hR14</i>	In ₂ S ₄ Zn	14	3
152	<i>hR14</i>	Mo ₃ Se ₄	3	3
176	<i>hR14</i>	Pd ₄ Pu ₃	4	3
185	<i>hR14</i>	S ₄ Ti ₃	8	2
188	<i>hR14</i>	S ₁₄ Ti ₁₁	8	2
3	<i>hR15</i>	Ag ₂ Cr ₇ S ₁₂	6	E
18	<i>hR15</i>	Al ₃₁ Cu ₁₆ Ni ₄	8	Poly
43	<i>hR15</i>	B ₁₃ C ₂	4	3
82	<i>hR15</i>	CeMo ₆ S ₈	4	4
104	<i>hR15</i>	Er ₃ Ni ₂	4	3
147	<i>hR15</i>	Mo ₆ PbS ₈	4	4
69	<i>hR16</i>	BiMn ₃	4	3
77	<i>hR16</i>	CSi	16	4
120	<i>hR16</i>	Ga ₃ Pu	4	2
132	<i>hR16</i>	InMg ₃	8	E
141	<i>hR16</i>	K ₃ SbSe ₄	4	3
153	<i>hR16</i>	N ₂	2	E
170	<i>hR16</i>	OZr ₃	5	E
29	<i>hR17</i>	As ₅ Fe ₁₀ Ru ₂	9	Poly
72	<i>hR17</i>	Bi ₈ Se ₉	9	1
101	<i>hR17</i>	Cu ₂ P ₂ Yb	9	Poly
150	<i>hR17</i>	Mo ₆ S ₈ Sn	5	E
171	<i>hR17</i>	P ₂ Pd ₁₅	5	4
49	<i>hR18</i>	B ₂ Co ₃ Zr	5	4
85	<i>hR18</i>	Co ₇ Er ₂	7	3
59	<i>hR19</i>	B ₆ Ni ₁₂ Sr	4	4
67	<i>hR19</i>	Be ₁₇ Nb ₂	5	4
169	<i>hR19</i>	O ₁₂ Pr ₇	4	E
194	<i>hR19</i>	Th ₂ Zn ₁₇	5	4
20	<i>hR20</i>	Al ₃ He	6	2
86	<i>hR20</i>	Co ₄ Fe ₄ Th	6	E
117	<i>hR20</i>	Ga ₁₄ Li ₃	4	3
126	<i>hR20</i>	H ₂ HoNi ₃	7	E
172	<i>hR20</i>	P ₃ Pd ₇	8	Poly
11	<i>hR21</i>	AlB ₄₀ C ₄	5	E
14	<i>hR21</i>	Al ₆ C ₃ N ₂	11	E
83	<i>hR21</i>	Ce ₇ O ₁₂	5	E
107	<i>hR21</i>	FeMo ₁₂ S ₁₆ Sn ₂	5	Poly
75	<i>hR22</i>	C ₂ Mn ₁₇ Pr ₂	6	E
114	<i>hR22</i>	Ga	5	4
144	<i>hR22</i>	Li ₅ Na ₂ Sn ₄	11	4
181	<i>hR22</i>	Rh ₃ ScSi ₇	4	4
186	<i>hR22</i>	S ₁₁ Ti ₈	12	2
190	<i>hR22</i>	Sb ₃ Zn ₄	3	3
128	<i>hR23</i>	HP ₄ Pd ₃₀	6	E
1	<i>hR24</i>	AgAsS ₂	4	2
81	<i>hR24</i>	Ce ₅ Co ₁₉	9	Poly
131	<i>hR24</i>	HgMg ₃	7	4
26	<i>hR25</i>	As ₄ Cu ₆ Hg ₃ S ₁₂	9	2
17	<i>hR26</i>	Al ₈ Cr ₅	9	2
22	<i>hR26</i>	AlPd	6	2
28	<i>hR26</i>	As ₆ Cu ₇ Se ₁₃	10	1

(continued)

TABLE 2. (continued)

No.	Pearson symbol	Structure type	No. of point sets	No. of AETs
96	<i>hR26</i>	Cu ₇ Hg ₆	9	Poly
103	<i>hR26</i>	Cu ₉ S ₅	14	E
142	<i>hR26</i>	Li ₅ Mo ₉ S ₁₂	5	E
146	<i>hR26</i>	Mo ₃ NiS ₄	5	E
179	<i>hR27</i>	Pd ₂₀ Sb ₇	6	3
189	<i>hR27</i>	STl ₂	9	E
32	<i>hR28</i>	As ₄ Pb ₉ S ₁₅	8	E
93	<i>hR28</i>	CsMo ₆ Se ₇	6	Poly
168	<i>hR28</i>	O ₅ P ₂	6	E
15	<i>hR29</i>	Al ₈ C ₃ N ₄	15	E
44	<i>hR29</i>	B ₁₉ C	6	E
41	<i>hR31</i>	B ₁₂ Ba ₇ Ir ₁₂	6	Poly
64	<i>hR31</i>	Ba ₂ NbS ₅	8	E
87	<i>hR32</i>	Co ₂ Ge ₃ S ₃	12	2
174	<i>hR32</i>	P ₁₆ Si ₉ Sn ₄	12	4
24	<i>hR34</i>	Al ₇ Te ₁₀	8	3
42	<i>hR34</i>	B ₆ Ba ₂ Ni ₉	4	3
105	<i>hR38</i>	Eu ₂ Re ₆ S ₁₁	5	4
123	<i>hR38</i>	Ge ₃ La ₄ S ₁₂	7	4
173	<i>hR38</i>	P ₁₃ Re ₆	7	3
6	<i>hR42</i>	AgMg ₅ Zn ₉	15	2
148	<i>hR42</i>	Mo ₉ Rb ₂ Se ₁₀	9	Poly
9	<i>hR44</i>	Al ₃ Au ₈	7	Poly
74	<i>hR44</i>	C ₄ HgN ₄ Rb ₂	7	E
139	<i>hR44</i>	In ₃ Yb ₈	7	Poly
151	<i>hR44</i>	Mo ₉ Si ₁₁ Tl ₂	10	4
177	<i>hR44</i>	Pd ₈ Sb ₃ - a	12	Poly
178	<i>hR44</i>	Pd ₈ Sb ₃ - b	24	Poly
5	<i>hR46</i>	Ag ₈ GeTe ₆	18	E
122	<i>hR49</i>	Ga ₄₁ V ₈	11	Poly
84	<i>hR53</i>	Co ₅ Cr ₂ Mo ₃	11	4
78	<i>hR62</i>	CSi	62	E
133	<i>hR72</i>	In ₂ Mo ₁₅ Se ₁₉	9	Poly
134	<i>hR73</i>	In ₄ SSe ₂ Te ₃	15	E
180	<i>hR92</i>	Re ₂₅ Zr ₂₁	10	3
46	<i>hR96</i>	B ₈ Ce ₁₅ N ₂₅	10	E
40	<i>hR105</i>	B	15	4
38	<i>hR111</i>	B	16	Poly
12	<i>hR113</i>	AlB ₅₂ Cu	17	E
52	<i>hR113</i>	B ₄₉ Fe	17	E
56	<i>hR115</i>	B ₂₃ Mn	18	E
61	<i>hR119</i>	B ₂₈ Sc	18	E
63	<i>hR119</i>	B ₅₁ Zr	18	E
118	<i>hR120</i>	Ga ₁₃ Na ₇	18	Poly
62	<i>hR121</i>	B ₂₅ Zn	19	E
50	<i>hR133</i>	B ₂₃ Cu	20	E
51	<i>hR133</i>	B ₂₈ Cu	20	E
10	<i>hR137</i>	AlB ₃₁	19	E
115	<i>hR138</i>	Ga ₅₀ K ₄ Na ₁₃	20	Poly
39	<i>hR141</i>	B	20	E
58	<i>hR143</i>	B ₉₇ Ni ₂	20	E
54	<i>hR155</i>	B ₉₀ Ge	22	E
16	<i>hR168</i>	AlCa ₃ Cd ₁₇	60	E
195	<i>hR16</i>	Ga ₇ Rb	4	4

E, excluded.

lead to too short (long) interatomic distances. We will show later on that it is possible to make a differentiation between structure types wherein the improbable in-

teratomic distances are physically impossible and structure types wherein the improbable interatomic distances can occur. Thus in total we excluded, after analysing all 195 structure types, 51 structure types for the reasons given above.

This left us with 144 structure types representing 1324 compounds and 6356 atomic environments (point sets). Our analysis was performed after the transformation of the data to the standard setting of the *International Tables for Crystallography*, Vol. A [5] and after comparing each entry with the original publication in order to prevent transcription errors.

Our aim by using this atomic environment analysis is to find answers to the following questions.

- (1) Which structure types are most likely to be correct?
- (2) Which structure types are related?
- (3) Which kinds of atomic environments are realized?
- (4) Which as yet unknown rules relates the nature of the constituents of a compound to its crystal structure?

In Section 2 we briefly recapitulate our method for defining an atomic environment type (AET).

Section 3 gives the observed atomic environment types and with the aid of some examples we show that incorrect structure determinations can lead to the re-actualization of incorrect atomic environments.

In Section 4 the results of the observed coordination types are briefly discussed and compared with results of other investigations.

Relations between the rhombohedral structure types are given in Section 5.

In Section 6 the structure types with improbable interatomic distances are discussed in detail and we show, with examples, that in some cases it is possible to redescribe the structure type in such a way that the resulting observed atomic environments are correct.

2. Classification of crystal structures based on atomic environments

A crystal structure is completely determined by the following data:

- (1) chemical formula,
- (2) space group and unit cell dimensions,
- (3) coordinates of the point sets (atomic positions) and their occupancy.

These characteristics lead to a fairly large number of different structure types (nearly 2800 types are listed in ref. 4, including the rhombohedral structure types), which makes it almost impossible to see connections or even to detect identities. About half of these structure types are described and geometrically depicted in the *Atlas of Crystal Structure Types for Intermetallic Phases* [6]. In this atlas we give for each structure type detailed

crystallographic data, a three-dimensional drawing of the unit cell, the cell content and two projections of the cell and for each atom in the asymmetrical unit the coordinates and drawings of the coordination polyhedra (atomic environments).

The remaining structure types were excluded from the atlas [6] for the following reasons:

- (1) all oxides with no intermetallic compounds,
- (2) incomplete structure types, *i.e.* if one of the atoms is not refined,
- (3) structure types with more than 20 point sets,
- (4) structure types with physically improbable interatomic distances,
- (5) structure types with either dumb-bells or dipoles.

It is obvious that on these grounds we excluded, apart from the incorrect structure types, also the structures with mainly ionic and/or covalent bonds between the atoms.

The aim of the concept described more extensively in ref. 1 and briefly recapitulated hereafter is to define the AEs as clearly as possible so that we will be able to group them into distinct AETs.

We defined an AE using the Brunner-Schwarzenbach method [7], in which all interatomic distances between an atom and its neighbours are plotted in a next-neighbour histogram as shown in Fig. 1a. In most cases a clear maximum gap is revealed, as can be seen in Fig. 1a. All atoms to the left of this maximum gap belong to the AE of the central atom. This rule is called the maximum gap rule and the AE of Fig. 1b is constructed according to this rule with the atoms to the left of the maximum gap. The AE environment shown in Fig. 1b is a truncated hexagonal eclipsed bipyramid, also called a twinned cubo-octahedron or an anticubo-octahedron [8, 9], and is found in hexagonal closed-packed structures. The structure types considered in ref. 4 are analysed according to this rule only and therefore there may be some differences between the analysis in this investigation and the AE depicted in the atlas.

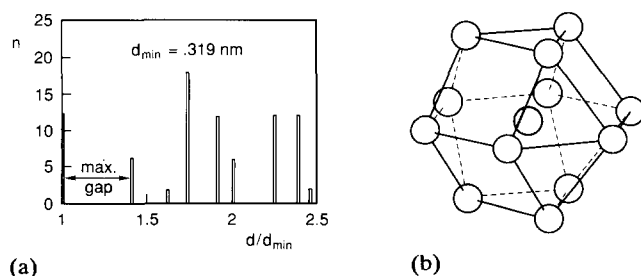


Fig. 1. (a) A typical example of a next-neighbour histogram and (b) the AE constructed with the atoms before the maximum gap in this histogram. The AE shown is the short-range atomic arrangement as observed in h.c.p. structures and is called the twinned cubo-octahedron.

In those cases where this rule leads to AEs with not only the central atom enclosed or to AEs with atoms on one (or more) of the faces of the coordination polyhedron, we defined the maximum convex volume rule. This rule is defined as the maximum volume around only one central atom enclosed by convex faces, with all the coordinating atoms lying at the intersections of at least three faces. This rule was also used in those cases where no clear maximum gap was detectable. In those cases where two (or more) equal or practically equal maximum gaps were observed, we kept the number of different AETs in a structure type as small as possible.

The AETs are characterized using the codes explained in refs. 1 and 10. The code of the AE shown in Fig. 1b is $12^{(2,2)}$, which is the same as the code for the cubo-octahedron, the latter being found in cubic closed-packed structures.

3. Observed atomic environment types

Using the rules given above, we have analysed all 144 rhombohedral intermetallic structure types. Our approach leads to conventional atomic environment types for most metals or alloys. However, in combinations of metals with p-elements on the right of the Zintl line or in combinations with hydrogen we sometimes obtained irregular AETs (IAETs). We consider normal AETs as environment types which can be visualized by coordination polyhedra and IAETs as environment types which cannot be described as a convex volume.

Our analysis showed that the 144 structure types with 1324 compounds have 6356 AEs (point sets) which belong to 67 distinct AETs. Of those AEs, 71% belong to one of the 14 most frequently occurring AETs shown in Fig. 2. AETs were added to this list when they were observed in at least 10 different structure types.

The remaining 53 normal AETs and IAETs are shown in Fig. 3. The 67 distinct high symmetry AETs were derived from 251 observed related AEs. This reduction was possible since we assigned the AEs with the lower symmetry code to the AEs with the highest symmetry code as explained in ref. 1. In Figs. 2 and 3 these 67 AETs and IAETs are listed together with their codes and labels. In ref. 1 the AETs were labelled by a capital character for the most frequently occurring AETs, by a number for the remaining AETs and the IAETs were labelled by a small character. This labelling system can, although it is in itself correct, easily lead to confusion when we combine the results from the "cubic" analysis [1] with the results from this analysis. Therefore we changed the labelling system of the AETs to labels which are a combination of the coordination number (CN) and a character, *e.g.* the icosahedron (old label K) is now labelled 12-a; the IAETs are also given by

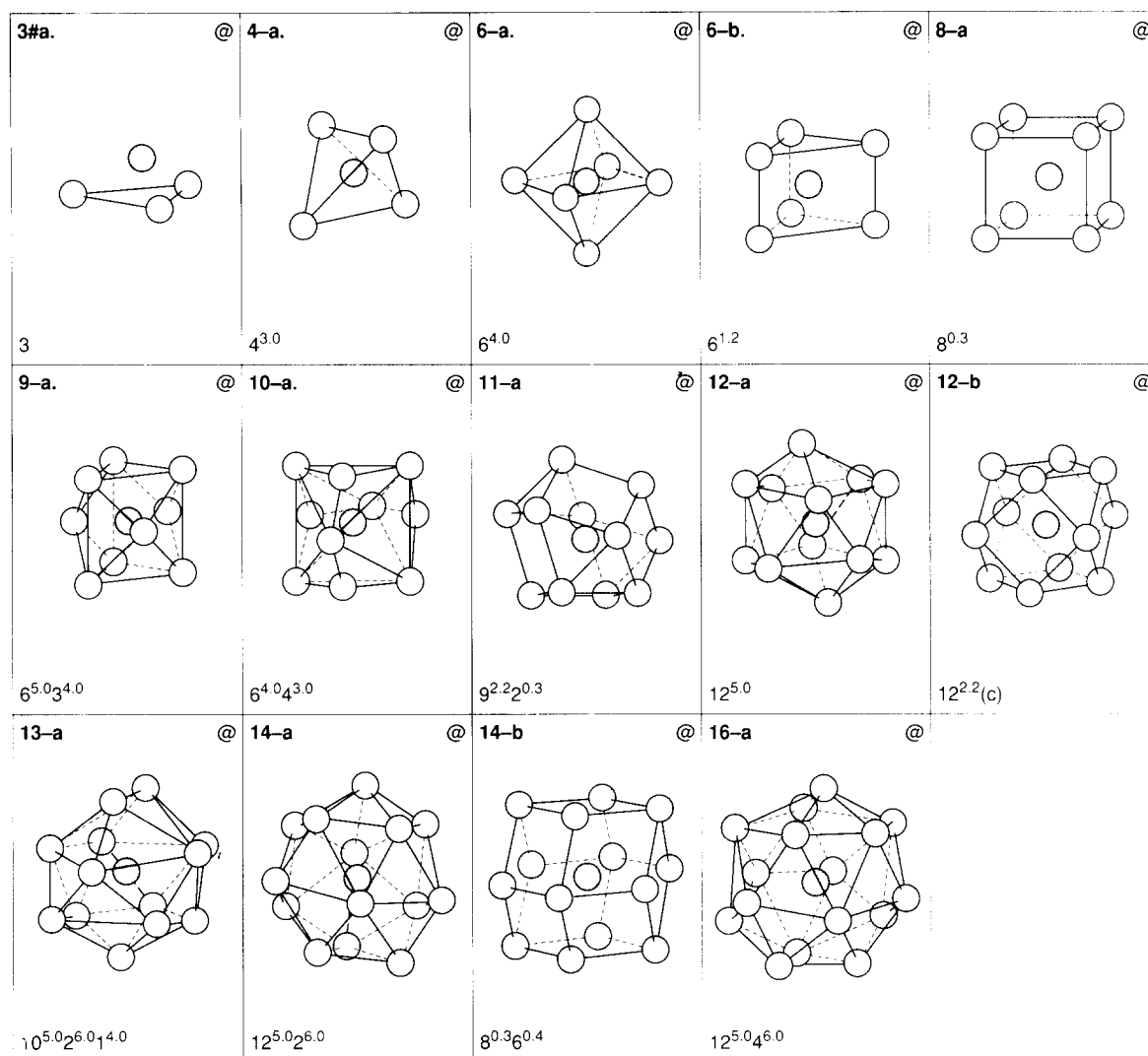


Fig. 2. The 14 most frequently occurring AETs with their polyhedron codes (lower left corner of each box). In the upper left corner of each box the assigned labels are given, consisting of the coordination number and a letter (a, b, ...) separated by a - for a normal AET and a # for an irregular AET. With an @ in the upper right corner we mark the AETs which are also observed in the cubic structure types.

the CN and a character but they are separated by a #, e.g. the loose triangle (old label d) is now labelled 3#a.

In Appendix A we list the observed AETs in the cubic symmetry with in the first column the old label and in the second column the new label; an @ is added to the label (in the third column) for the AETs which are also observed in the structure types with rhombohedral symmetry. In addition, we give the number of times that the AET is observed in the structure types in respectively the single- to poly-environment groups and in the last column the total. In Appendix B the number of point sets for each AET is given in the same manner.

In Fig. 4 the distribution frequency observed for the 14 most frequently occurring AETs in the rhombohedral

structure types is plotted. When compared with our results from the cubic structure types [1], we see some similarities as well as some differences. As in the cubic case, the AETs with even coordination numbers are greatly preferred; the tetrahedron, the octahedron and the icosahedron are observed more often than the other AETs.

Remarkably, an IAET had to be added to the list because it appeared in many rhombohedral structure types. This IAET is the loose triangle 3#a (Fig. 2) and it is observed mainly in combinations of metals with sulphur, selenium and tellurium.

The loose triangle appears mainly in so-called layered structures. For example, in *hR3* MoS₂ the molybdenum atomic environment is an anticubo-octahedron consisting of six sulphur and six molybdenum atoms, while

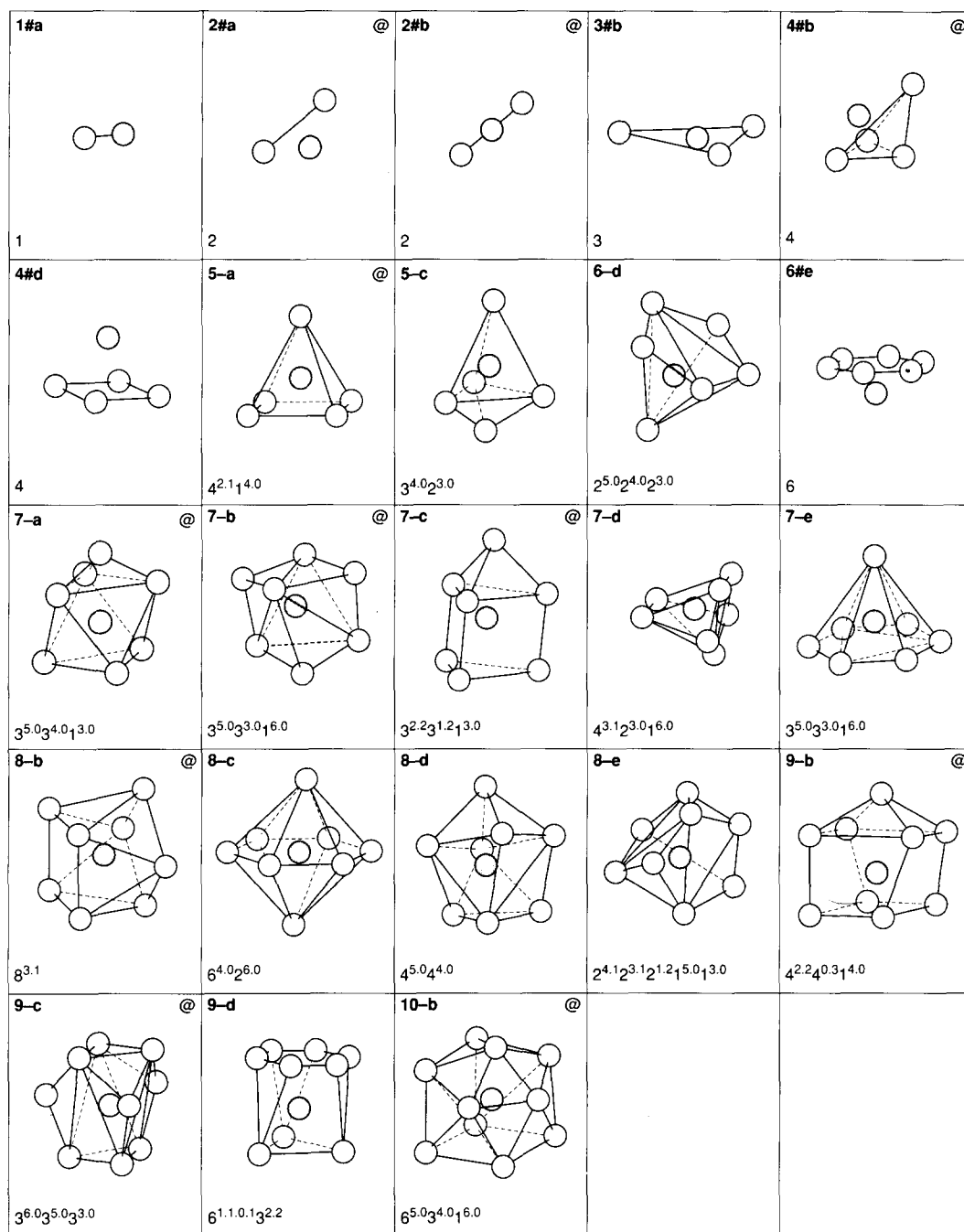


Fig. 3.

(continued)

both sulphur atoms have three molybdenum atoms as their nearest neighbours; see Figs. 5a–5f for the atomic environments and the corresponding next-neighbour histograms (NNHs).

In Fig. 6a the NNH of one of the sulphur atoms is given and apart from the maximum gap three other gaps are defined (b–d respectively). We show in the Figs. 6b–6d the “polyhedrons” belonging to these gaps and we observe that the “polyhedron” constructed with

the 10 atoms of gap b (see Fig. 6b) is a loose 10-atom body, meaning that all 10 atoms are situated on one side of the sulphur atom. Including the next three neighbouring atoms belonging to gap c (see Fig. 6c) gives a very distorted convex polyhedron and constructing a polyhedron with the 16 atoms belonging to gap d (see Fig. 6d) gives a polyhedron with three atoms (shaded in Fig. 6d) situated exactly on the edges of the polyhedron.

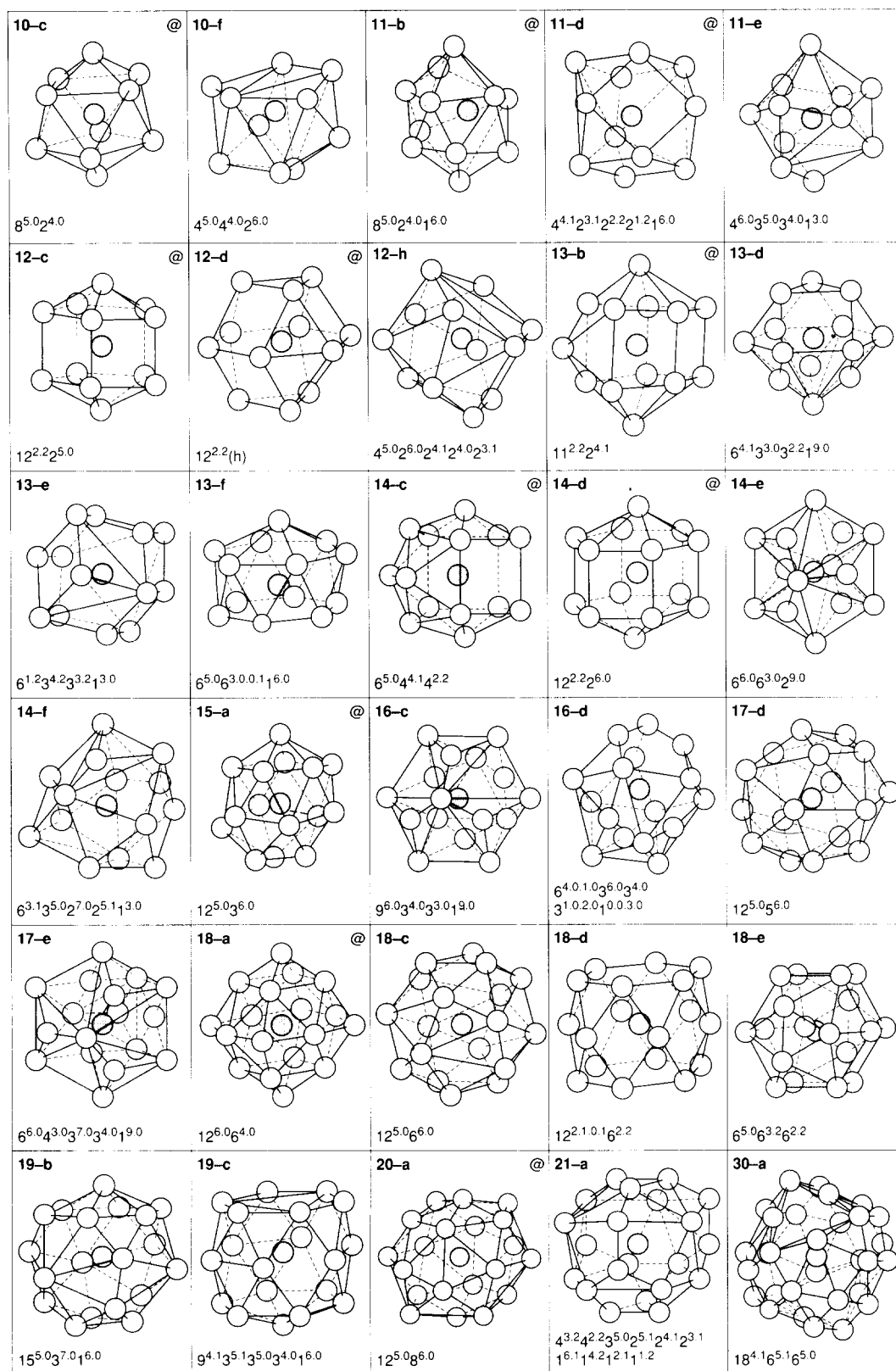


Fig. 3. The remaining 53 AETs and IAETs with their polyhedron codes (lower left corner of each box). In the upper left corner of each box the assigned labels are given, consisting of the coordination number and a letter (a, b, ...) separated by a - for a normal AET and a # for an irregular AET. With an @ in the upper right corner we mark the AETs which are also observed in the cubic structure types.

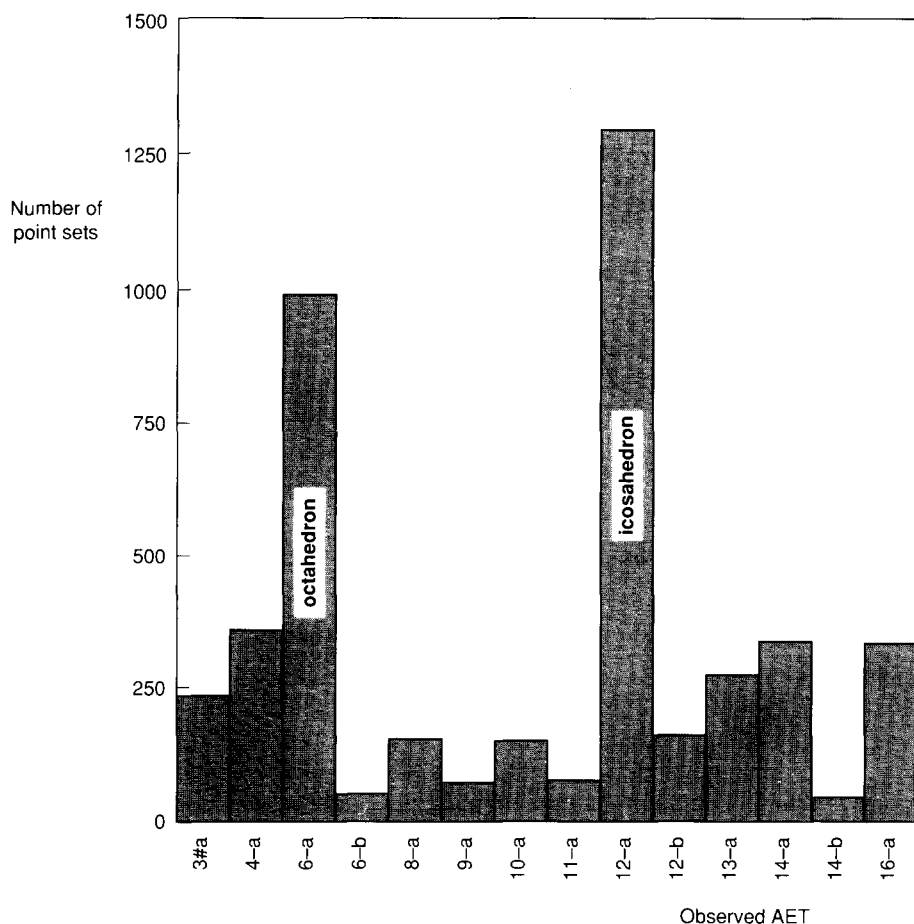


Fig. 4. A frequency plot of the 14 most frequently occurring AETs.

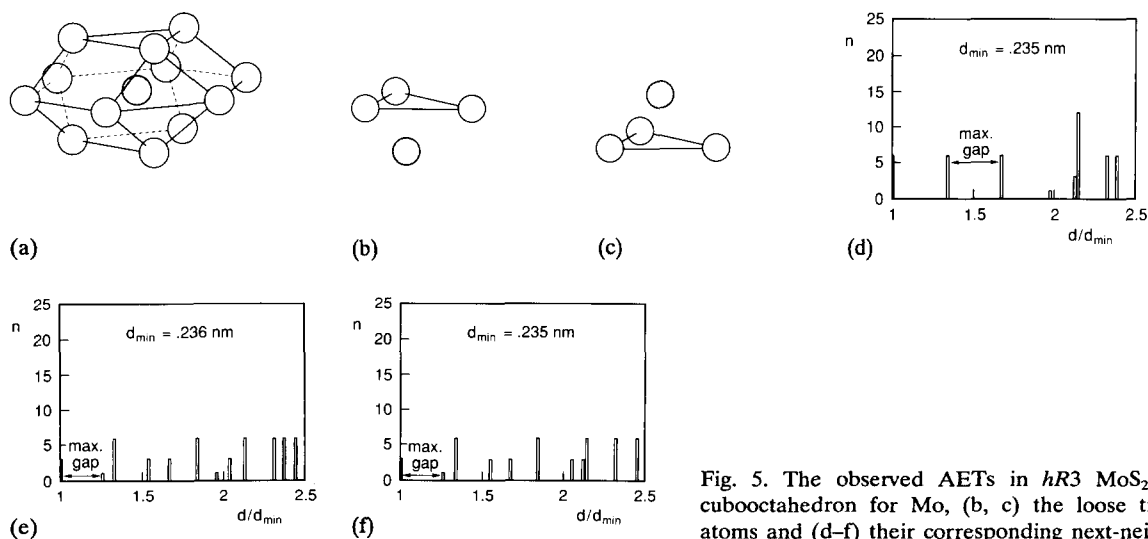


Fig. 5. The observed AETs in $hR3$ MoS_2 ; (a) the twinned cubooctahedron for Mo, (b, c) the loose triangle for both S atoms and (d-f) their corresponding next-neighbour histograms.

With this example we demonstrate that in some structures the preferable atomic environment is not always a complete polyhedron but that an irregular atomic environment is sometimes a better choice, especially in these layered structures.

As in the cubic symmetry, it is not possible to decide whether some of these odd AETs are real or a consequence of the inaccuracy of the structure determination. Although in the following example the analysis did not lead to new AETs, the inconsistency sometimes

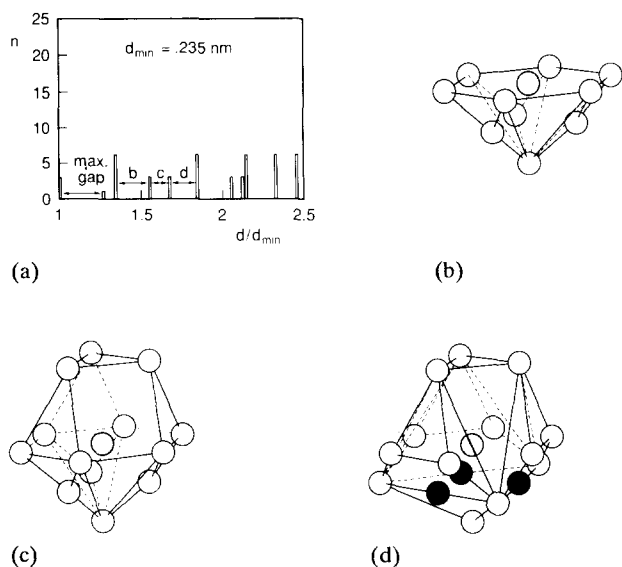


Fig. 6. (a) The NNH for one of the sulphur atoms in *hR3* MoS₂ and (b-d) the AEs constructed with the atoms belonging to one of the shown gaps, with (b) 10, (c) 13 and (d) 16 atoms respectively.

observed in structure determinations is clearly demonstrated.

In the system Pd-Sb two structure determinations are published, both with the composition Pd₈Sb₃, numbers 177 and 178, both solutions having the rhombohedral symmetry and as Pearson symbol *hR44* (crystallographic data of both compounds in Table 3), with respectively 12 or 24 atoms in the asymmetric unit. In the structure description with 12 point sets five different AETs are observed, while in the description with 24 point sets seven AETs are observed (see Table 8 with the poly-environment types).

It is fairly obvious that in the example given one of the solutions is incorrect or, more probably, in the latter solution, which has the lowest symmetry, the structure is refined in the wrong space group (see also Table 11). Although it is not the direct purpose of this study, it is in this example quite obvious that we think that the description with the highest symmetry is the best model for describing this structure type.

TABLE 3. Crystallographic data for the structure type *hR44* Pd₈Sb₃ refined in two space groups (161 and 146)

177 <i>hR44</i> Pd ₈ Sb ₃ - a						178 <i>hR44</i> Pd ₈ Sb ₃ - b					
Space group No. 161						Space group No. 146					
<i>R3c</i>						<i>R3</i>					
<i>a</i> = 0.76152 nm						<i>a</i> = 0.759 nm					
<i>c</i> = 4.3032 nm						<i>c</i> = 4.32 nm					
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>
Pd1	6 <i>a</i>	0	0	0.7301	1	Pd1	3 <i>a</i>	0	0	0.142	1
Pd2	6 <i>a</i>	0	0	0.3864	1	Pd2	3 <i>a</i>	0	0	0.202	1
Pd3	6 <i>a</i>	0	0	0.0104	1	Pd3	3 <i>a</i>	0	0	0.365	1
Pd4	6 <i>a</i>	0	0	0.6680	1	Pd4	3 <i>a</i>	0	0	0.490	1
Sb1	6 <i>a</i>	0	0	0.7921	1	Pd5	3 <i>a</i>	0	0	0.646	1
Sb2	6 <i>a</i>	0	0	0.1060	1	Pd6	3 <i>a</i>	0	0	0.707	1
Sb3	6 <i>a</i>	0	0	0.4487	1	Pd7	3 <i>a</i>	0	0	0.860	1
Pd5	18 <i>b</i>	0.5882	0.9139	0.0000	1	Pd8	3 <i>a</i>	0	0	0.989	1
Pd6	18 <i>b</i>	0.3495	0.0103	0.0325	1	Sb1	3 <i>a</i>	0	0	0.081	1
Pd7	18 <i>b</i>	0.7320	0.0026	0.0626	1	Sb2	3 <i>a</i>	0	0	0.261	1
Pd8	18 <i>b</i>	0.3638	0.0023	0.0976	1	Sb3	3 <i>a</i>	0	0	0.427	1
Sb4	18 <i>b</i>	0.6774	0.9782	0.1323	1	Sb4	3 <i>a</i>	0	0	0.583	1
						Sb5	3 <i>a</i>	0	0	0.769	1
						Sb6	3 <i>a</i>	0	0	0.925	1
						Pd9	9 <i>b</i>	0.250	0.010	0.038	1
						Pd10	9 <i>b</i>	0.735	0.008	0.536	1
						Pd11	9 <i>b</i>	0.651	0.004	0.074	1
						Pd12	9 <i>b</i>	0.358	0.997	0.567	1
						Pd13	9 <i>b</i>	0.306	0.001	0.105	1
						Pd14	9 <i>b</i>	0.694	0.002	0.609	1
						Pd15	9 <i>b</i>	0.640	0.017	0.141	1
						Pd16	9 <i>b</i>	0.430	0.079	0.642	1
						Sb7	9 <i>b</i>	0.657	0.006	0.006	1
						Sb8	9 <i>b</i>	0.360	0.010	0.506	1

B, multiplicity and Wyckoff letter; *N*, occupancy.

4. Observed coordination types

Before we give the classification we will introduce the term coordination type. In our classification, structure types belong to a certain coordination type when they have the same number and kinds of AETs.

The 144 analysed structure types of Table 1 can be divided into five groups according to the number of different AETs.

(1) Single-environment structures, *i.e.* all atoms have the same AET. This group of 14 structure types containing 257 representatives with a total of 762 point sets can be subdivided into six coordination types.

(2) Two-environment structures, *i.e.* each of the atoms has one of the two AETs. This group of 39 structure types containing 203 representatives with a total of 766 point sets can be subdivided into 19 coordination types.

(3) Three-environment structures, *i.e.* each of the atoms has one of the three AETs. This group of 36 structure types containing 327 representatives with a total of 1623 point sets can be subdivided into 24 coordination types.

(4) Four-environment structures, *i.e.* each of the atoms has one of the four AETs. This group of 34 structure types containing 456 representatives with a total of

2244 point sets can be subdivided into 29 coordination types.

(5) Poly-environment structures combining more than four AETs. This group of 21 structure types (with 20 coordination types) contains 81 representatives with a total of 961 point sets.

In Tables 4–8 the structures are arranged according to the number of environments, from single-environment (Table 4) to poly-environment (Table 8) structures.

In the single-environment group we observed six coordination types, giving a reduction of 57% compared with the 14 structure types. Almost the same reduction is observed in the two-environment group, namely 51%; the reduction in the three-environment group is 31%, in the four-environment group 15% and in the poly-environment group 5%.

In Table 9 we list the observed AETs in the rhombohedral symmetry with in the first column the label (an @ is added to this label in the second column when the AET was also observed in the cubic structure types), in the next five columns the number of times the AET is observed in a structure type in respectively the single- to poly-environment groups and in the last column the total. In Table 10 we list in the same manner the number of times an AET is observed on a point set.

TABLE 4. Structure types belonging to the single-environment group ordered according to coordination types with increasing coordination numbers

No.	Pearson symbol	Structure type	No. of point sets	No. of compounds	Coordination number	Most frequently occurring Atomic Environment Types												Remaining Atomic Environment Types		Remarks	
						3#a	4-a	6-a	6-b	8-a	9-a	10-a	11-a	12-a	12-b	13-a	14-a	14-b	16-a		AET
191	hR6	Se	1	2	2														2#a		
28	hR26	As ₆ Cu ₇ Se ₁₃	10	1	4		X														
25	hR2	As	1	20	6			X													
90	hR4	CrNaS ₂	3	144	6			X													
73	hR5	Bi ₂ Te ₃	3	52	6			X													
71	hR7	Bi ₂ Se ₄	4	18	6			X													
192	hR8	Se ₄ Zr ₃	4	6	6			X													
68	hR11	Bi ₂ Ge ₃ Te ₆	11	1	6			X													
72	hR17	Bi ₈ Se ₉	9	1	6			X													
129	hR1	Hg	1	5	12								X								
130	hR2	HgIn	2	2	12								X								
36	hR6	Au ₅ Sn	4	1	12													12-d			
116	hR5	Ga ₂ Li ₃	3	3	14												X				
145	hR7	Li ₇ Si ₃	4	1	14												X				
14 structure types			257 compounds												9			13	4	2	point sets 762

TABLE 5. Structure types belonging to the two-environment group ordered according to coordination types with increasing coordination numbers. F-K designates a Frank-Kasper structure type

No.	Pearson symbol	Structure type	No. of point sets	No. of compounds	Coordination numbers	Most frequently occurring Atomic Environment Types													Remaining Atomic Environment Types		Remarks		
						3#a	4-a	6-a	6-b	8-a	9-a	10-a	11-a	12-a	12-b	13-a	14-a	14-b	16-a	AET		IAET	
76	hR8	CNi ₃	2	3	2/6															2#a			
121	hR4	GaSe	4	2	3/4																		
2	hR14	Ag ₃ AsS ₃	3	4	3/4																		
1	hR24	AgAsS ₂	4	2	3/4																		
25	hR25	As ₄ Cu ₆ Hg ₃ S ₁₂	9	2	3/4																		
30	hR11	As ₂ Ge ₃ Te ₆	6	1	3/6																		
31	hR13	As ₂ Ge ₄ Te ₇	7	1	3/6																		
149	hR3	MoS ₂	3	18	3/12															12-d			
154	hR3	N ₂ W	2	12	3/14															14-e			
175	hR8	P ₃ Sn	2	2	4/6																		
21	hR10	Al ₂ O ₃	2	11	4/6																		
140	hR12	Ir ₃ Se ₈	4	1	4/6																		
87	hR32	Co ₂ Ge ₃ S ₃	12	2	4/6																		
60	hR14	B ₆ P	3	6	4/6															6-d			
165	hR4	NiTe	2	1	4/7															7-c			
161	hR6	NiS	2	2	5/7															5-a; 7-b			
159	hR4	NbS ₂	4	9	6/6																		
184	hR6	STi	4	1	6/6																		
187	hR8	S ₁₂ Ti ₇	5	10	6/6																		
185	hR14	S ₄ Ti ₃	8	1	6/6																		
188	hR14	S ₁₄ Ti ₁₁	8	1	6/6																		
186	hR22	S ₁₁ Ti ₈	12	1	6/6																		
37	hR12	B	2	1	6/7															6-d; 7-d			
162	hR5	Ni ₃ S ₂	2	3	6/8																		
164	hR5	Ni ₃ Se ₂	2	1	6/8																		
4	hR6	AgCrSe ₂	4	14	6/10															10-b			
166	hR7	Ni ₂ Ti	4	1	8/10															8-c; 1-b			
193	hR3	Sm	2	31	12/12															12-d			
65	hR12	BaPb ₃	4	26	12/12															12-d			
120	hR16	Ga ₃ Pu	4	3	12/12															12-d			
20	hR20	Al ₃ Ho	6	11	12/12															12-d			
17	hR26	Al ₉ Cr ₅	9	6	12/13																		
112	hR6	Fe ₂ Tb	3	3	12/16																F-K		
124	hR6	GeRh ₃ Y ₂	3	5	12/16																F-K		
6	hR42	AgMg ₅ Zn ₉	15	1	12/16																F-K		
7	hR8	AgNb ₄ S ₈	4	1	13/14															13-d; 14-e			
8	hR8	AgS ₃ Ta ₄	4	1	13/14															13-d; 14-e			
119	hR14	Ga ₄ Pd ₇ Zn ₃	6	1	13/14															13-b;			
22	hR26	AlPd	6	1	13/14															13-c;			
39 structure types				203 compounds		70	64	147	40	4				60	133	18			4	15	208	3	point sets 766

TABLE 6. Structure types belonging to the three-environment group ordered according to coordination types with increasing coordination numbers. F-K designates a Frank-Kasper structure type

No.	Pearson symbol	Structure type	No. of point sets	No. of compounds	Coordination numbers	Most frequently occurring Atomic Environment Types													Remaining Atomic Environment Types		Remarks		
						3#a	4-a	6-a	6-b	8-a	9-a	10-a	11-a	12-a	12-b	13-a	14-a	14-b	16-a	AET		IAET	
33	hR7	AsSe ₃ Tl ₃	3	5	1/3/14	X														14-f	1#a		
141	hR16	K ₃ SbSe ₄	4	1	1/4/14		X															1#a	
24	hR34	Al ₇ Te ₁₀	8	1	2/3/4	X	X															2#a	
43	hR15	B ₁₃ C ₂	4	3	2/4/6		X													6-d		2#b	
69	hR16	BiMn ₃	4	1	2/12/14								X					X				2#a	
138	hR5	In ₂ Se ₃	5	5	3/4/6	X	X	X															
135	hR7	In ₂ S ₄ Zn	7	16	3/4/6	X	X	X	X														
106	hR9	Fe ₂ Ga ₂ S ₅	5	1	3/4/6	X	X	X															
137	hR9	In ₂ S ₅ Zn ₂	9	1	3/4/6	X	X	X	X														
108	hR10	FePSe ₃	3	8	3/4/6	X	X	X	X														
109	hR10	FePSe ₃	6	2	3/4/6	X	X	X	X														
182	hR11	Rh ₃ Se ₈	3	3	3/4/6	X	X	X															
79	hR13	C ₅ Ti ₈	5	1	3/4/6	X	X	X															
136	hR14	In ₂ S ₄ Zn	14	1	3/4/6	X	X	X															
152	hR14	Mo ₃ Se ₄	2	23	3/4/10	X	X	X												10-b			
183	hR6	S ₂ Ta	6	1	3/6/6	X	X	X	X														
91	hR9	Cr ₇ Na ₂ Se ₁₂	5	1	3/6/14	X		X												14-e			
158	hR4	NaS ₄ Ti ₂	4	8	3/6/16	X	X	X												16-d			
13	hR7	Al ₄ C ₃	4	2	4/5/6	X	X	X												5-a			
190	hR22	Sb ₃ Zn ₄	3	2	4/5/6	X	X	X												5-a			
173	hR38	P ₁₃ Re ₅	7	1	4/8/9	X			X											8-d			
47	hR13	B ₆ Co ₂ Pr ₅	5	3	5/6/14															5-c; 14-d		6#e	
100	hR9	CuNb ₆ S ₁₀	5	1	6/7/14			X												7-c; 14-e			
80	hR6	CaSi ₂	3	5	6/7/16		X	X												7-c; 16-c			
95	hR4	Cu ₂ GaSr	3	2	6/10/20		X	X		X										20-a			
111	hR10	Fe ₃ Sn ₂	3	2	6/11/15						X									15-a		6#e	
155	hR5	N ₆ W ₇	3	1	6/13/14		X													13-d; 14-e			
34	hR12	AuNa ₃ S ₂	3	1	7/8/14				X											7-a			
42	hR34	B ₆ Ba ₂ Ni ₉	4	1	7/8/15															7-b; 8-d; 15-a			
104	hR15	Er ₃ Ni ₂	4	20	9/14/16				X														
117	hR20	Ga ₁₄ Li ₃	4	1	10/10/14															10-b; 10-f			
179	hR27	Pd ₂₀ Sb ₇	6	2	12/13/16						X		X										
176	hR14	Pd ₄ Pu ₃	4	31	12/14/16						X		X	X									
180	hR92	Re ₂₅ Zr ₂₁	10	3	12/14/16						X	X	X	X									F-K
66	hR12	Be ₃ Nb	5	122	12/16/20						X	X	X	X						20-a			
85	hR18	Co ₇ Er ₂	7	45	12/16/20						X	X	X	X						20-a			
36 structure types			327 compounds			110	124	73	3	1	21	2	2	645	1	8	92	243	273		25	point sets 1623	

TABLE 7. Structure types belonging to the four-environment group ordered according to coordination types with increasing coordination numbers. F-K designates a Frank-Kasper structure type

No.	Pearson symbol	Structure type	No. of point sets	No. of compounds	Coordination numbers	Most frequently occurring Atomic Environment Types																Remaining Atomic Environment Types		Remarks
						3#a	4-a	6-a	6-b	8-a	9-a	10-a	11-a	12-a	12-b	13-a	14-a	14-b	16-a	AET	IAET			
77	hR16	CSi	16	1	1/4/4/7		X														7-e	1#a 4#b		
123	hR38	Ge ₃ La ₄ S ₁₂	7	11	1/4/7/9		X				X											7-b	1#a	
45	hR12	B ₂ CU	4	2	2/3/6/9			X														9-c	2#b 3#b	
48	hR13	B ₆ Co ₃ Tb ₄	5	21	2/5/6/7																	5-c; 7-a	2#b 6#e	
174	hR32	P ₁₆ Si ₉ Sn ₄	12	1	3/4/6/7	X	X	X														7-a		
105	hR38	Eu ₂ Re ₆ S ₁₁	5	4	3/4/9/14	X	X															9-b		
110	hR7	Fe ₃ S ₄	4	1	3/6/13/14	X			X													13-d; 14-e		
160	hR7	Ni ₃ Pb ₂ S ₂	4	19	3/8/10/12	X							X									8-c; 10-c		
163	hR7	Ni ₃ S ₂ Sn ₂	4	1	3/8/10/12	X						X										8-c; 10-c		
97	hR8	Cu ₃ K ₃ P ₂	4	3	3/12/14/18	X						X										14-c; 18-c		
82	hR15	CeMo ₆ S ₈	4	1	4/4/8/10		X			X		X											4#b	
147	hR15	Mo ₆ PbS ₈	4	115	4/4/8/10		X			X		X											4#b	
151	hR44	Mo ₉ S ₁₁ Tl ₂	10	2	4/4/8/10		X			X		X											4#b	
89	hR4	CrCuSe ₂	4	5	4/5/6/7		X		X													5-c; 7-a		
195	hR16	Ga ₇ Rb	4	1	4/6/7/21		X		X													7-d; 21-a		
92	hR10	Cr ₂ S ₃	4	6	4/6/8/13		X		X		X											13-d	4#b	
35	hR13	Au ₇ Rb ₄ Sn ₂	5	1	4/6/17/19		X		X													17-d; 19-b		
40	hR105	B	15	1	6/6/8/9		X		X													6-d; 8-e; 9-c		
114	hR22	Ga	5	1	6/8/10/12		X		X													8-e; 10-c; 12-h		
57	hR7	B ₃ Mo ₂	4	5	6/9/10/20		X			X												10-b; 20-a		
171	hR17	P ₂ Pd ₁₅	5	1	6/12/14/15				X			X										15-a		
102	hR12	Cu ₅ P ₄ Yb ₂	6	1	7/10/13/14					X												7-a; 13-e		
59	hR19	B ₆ Ni ₁₂ Sr	4	21	7/11/12/30					X		X										7-b; 30-a		
143	hR10	Li ₅ NaSn ₄	10	1	7/11/13/14					X												7-c; 13-b		
181	hR22	Rh ₃ ScSi ₇	4	2	8/9/9/18					X												8-e; 9-b; 18-c		
49	hR18	B ₂ Co ₃ Zr	5	2	9/13/14/20					X				X								20-a		
27	hR7	As ₂ Cu ₄ Na	4	4	10/13/14/20					X												13-e; 20-a		
19	hR9	Al ₄ Cu ₃ Zn	9	1	11/11/13/14					X												11-d; 13-b		
144	hR22	Li ₅ Na ₂ Sn ₄	11	1	11/12/13/14					X												13-b		
131	hR24	HgMg ₃	7	1	12/12/12/13					X		X										12-c; 13-b		
67	hR19	Be ₁₇ Nb ₂	5	5	12/13/14/19					X				X								19-c		
194	hR19	Th ₂ Zn ₁₇	5	160	12/13/14/19					X				X								19-c		
113	hR13	Fe ₇ W ₆	5	42	12/14/15/16					X				X								15-a	F-K	
84	hR53	Co ₅ Cr ₂ Mo ₃	11	12	12/14/15/16					X				X								15-a	F-K	
34 structure types			456 compounds			33	162	18	8	126	20	128	32	534	2	167	239	15	16	632	112	point sets 2244		

TABLE 8. Structure types belonging to the poly-environment group ordered according to coordination types with increasing coordination numbers

No.	Pearson symbol	Structure type	No. of point sets	No. of compounds	Coordination numbers	Most frequently occurring Atomic Environment Types											Remaining Atomic Environment Types		Remarks				
						3#a	4-a	6-a	6-b	8-a	9-a	10-a	11-a	12-a	12-b	13-a	14-a	14-b		16-a	AET	IAET	
133	hR72	In ₂ Mo ₁₅ Se ₁₉	9	10	3/4/9/10/11	X					X	X	X								4#b	5 AETs	
93	hR28	CsMo ₆ Se ₇	6	1	3/4/9/10/13	X					X	X									4#b	5 "	
148	hR42	Mo ₉ Rb ₂ Se ₁₀	9	1	3/4/10/12/13	X					X	X									4#b	5 "	
41	hR31	B ₁₂ Ba ₇ Ir ₁₂	6	1	4/4/5/17/18		X														5-c; 17-d; 18-c	4#d	5 "
96	hR26	Cu ₇ Hg ₆	9	1	4/7/8/9/9/12						X	X									7-a; 8-d; 9-b	4#b	6 "
38	hR111	B	16	24	6/6/7/8/9		X														6-d; 7-d; 8-e; 9-c		5 "
115	hR138	Ga ₅₀ K ₄ Na ₁₃	20	1	6/8/9/10/11 16/18/19/20						X	X									6-d; 8-d; 10-c; 11-b; 18-c; 19-b; 20-a		9 "
172	hR20	P ₃ Pd ₇	8	1	7/8/8/13/16						X	X									7-b; 8-b; 8-d		5 "
107	hR21	FeMo ₂ S ₁₆ Sn ₂	5	1	7/8/9/10/14						X	X									7-a; 8-d; 10-c		5 "
99	hR6	Cu ₃ NaTe ₂	6	1	7/9/10/11/17						X	X									7-c; 10-b; 11-e; 17-e		5 "
101	hR17	Cu ₂ P ₂ Yb	9	1	7/10/13/14/18						X	X									7-b; 13-e; 18-a		5 "
122	hR49	Ga ₄₁ V ₈	11	13	8/9/10/10/12/13						X	X									9-b; 10-b; 10-c		6 "
9	hR44	Al ₃ Au ₈	7	1	8/10/11/12/13						X	X									10-c		5 "
177	hR44	Pd ₈ Sb ₃ -a	12	9	8/10/11/12/13						X	X									10-c		5 "
139	hR44	In ₂ Yb ₅	7	2	8/10/11/12 13/14						X	X									10-c		6 "
178	hR44	Pd ₈ Sb ₃ -b	24	1	8/10/11/12 13/14/15						X	X									15-a		7 "
29	hR17	As ₅ Fe ₁₀ Ru ₂	9	5	9/10/11/12 14/15						X	X									10-b; 15-a		6 "
118	hR120	Ga ₁₃ Na ₇	18	1	10/11/13/16/18																10-b; 11-b; 13-f; 18-c		5 "
23	hR14	Al ₉ Sr ₅	6	1	10/12/14/16/18							X	X								10-b; 18-e		5 "
18	hR15	Al ₃₁ Cu ₄₆ Ni ₄	8	1	11/11/12/13/14						X	X									11-d; 13-b		5 "
81	hR24	Ce ₅ Co ₁₉	9	4	12/12/12/16 18/20						X	X									12-d; 18-d; 20-a		5 "
21	structure types			81	compounds	22	2	24		26	31	19	42	52	18	81	10	3	13	581		37	point sets 961

When for the single-environment group we combine our results with the results of ref. 1, the number of structure types increases to 40 but the number of coordination types only to 8. It is therefore to be expected that after completing the analysis of all crystal symmetries, the number of coordination types will be significantly lower than the number of structure types.

In the cubic case we found that 92% of the compounds crystallize with one, two or three AETs. In this analysis we observe that 94% of the compounds crystallize in structure types with one, two, three or four AETs (see Fig. 7). Remarkably, most compounds have four AETs,

meaning that in the rhombohedral case the structures are more complex than in the cubic case. In Table 7 it can be seen that two of the most "popular" rhombohedral structure types, *hR19* Th₂Zn₁₇ and *hR15* Mo₆PbS₈, belong to the four-environment group.

5. Related structure types

One of the main advantages of our analysis method is that it is easy to find relations between structures, which enable a differentiation to be made between three types of structural relations.

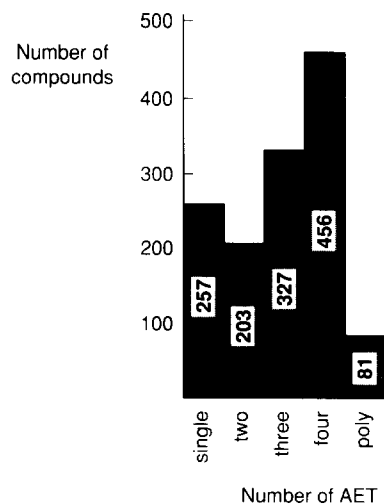


Fig. 7. Number of compounds vs. number of AETs per structure type for the 1324 rhombohedral compounds.

TABLE 9. Number of times an AET is observed in the rhombohedral structure types; an @ is added to the labels in the second column when the AET was also observed in the cubic structure types

New label	Cubic	Environment types					Total no. of structure types
		I	II	III	IV	Poly	
1#a				2	2		4
2#a	@	1	1	2			4
2#b	@			1	2		3
3#a	@		8	15	6	3	32
3#b					1		1
4-a	@	1	10	15	10	1	37
4#b	@			1	5	4	10
4#d			1		1	1	2
5-a	@			2			3
5-c				1	2	1	4
6-a	@	7	14	16	7	1	45
6-b	@		8	3	4		15
6-d			2	1	1	2	6
6#e				2	1		3
7-a	@			1	4	2	7
7-b	@		1	1	2	2	6
7-c	@		1	2	1	1	5
7-d			1		1	1	3
7-e					1		1
8-a	@		2	1	4	5	12
8-b	@					1	1
8-c			1		2		3
8-d				2		4	6
8-e					3	1	4
9-a	@			2	4	7	13
9-b	@				2	2	4
9-c	@				1	1	2
9-d					1		1
10-a	@			1	5	5	11
10-b	@		2	1	1	5	9
10-c	@			1	3	6	10

(continued)

TABLE 9. (continued)

New label	Cubic	Environment types					Total no. of structure types
		I	II	III	IV	Poly	
10-f				1			1
11-a	@			1	4	7	12
11-b	@					2	2
11-d	@				1	1	2
11-e					1	1	2
12-a	@		4	5	10	9	28
12-b	@	2	4	1	2	3	12
12-c	@				1		1
12-d	@	1	5			1	7
12-h					1		1
13-a	@		1	1	3	8	13
13-b	@		2		4	1	7
13-d			2	1	2		5
13-e					2	1	3
13-f						1	1
14-a	@			7	7	5	19
14-b	@	2	2		5	2	11
14-c	@				1		1
14-d	@			1			1
14-e			3	3	1		7
14-f				1			1
15-a	@			2	3	2	7
16-a	@		3	6	2	5	16
16-c				1			1
16-d				1			1
17-d					1	1	2
17-e						1	1
18-a	@					1	1
18-c					2	3	5
18-d						1	1
18-e						1	1
19-b					1	1	2
19-c					2		2
20-a	@			3	3	2	8
21-a					1		1
30-a					1		1

TABLE 10. Number of times an AET is observed on a point set in the rhombohedral structure types; an @ is added to the labels in the second column when the AET was also observed in the cubic structure types

New label	Cubic	Environment types					Total no. of point sets
		I	II	III	IV	Poly	
1#a				7	45		52
2#a	@	2	3	4			9
2#b	@			3	23		26
3#a	@		70	110	33	22	235
3#b					2		2
4-a	@	10	64	124	162	2	362
4#b	@			23	129	36	188
4#d						1	1
5-a	@		2	4			6
5-c				3	26	1	30

(continued)

TABLE 10. (continued)

New label	Cubic	Environment types					Total no. of point sets
		I	II	III	IV	Poly	
6-a	@	724	147	73	18	24	986
6-b	@		40	3	8		51
6-d			13	6	10	169	198
6#e				11	42		53
7-a	@			1	28	2	31
7-b	@		2	1	32	3	38
7-c	@		1	6	1	1	9
7-d			1		1	24	26
7-e					3		3
8-a	@		4	1	126	26	157
8-b	@					1	1
8-c			3		20		23
8-d				3		9	12
8-e					7	144	151
9-a	@			21	20	31	72
9-b	@				6	28	34
9-c	@				1	24	25
9-d					2		2
10-a	@			2	128	19	149
10-b	@		29	1	5	41	76
10-c	@			23	21	71	115
10-f				2			2
11-a	@			2	32	42	76
11-b	@					14	14
11-d	@				2	2	4
11-e						2	2
12-a	@		60	645	534	52	1291
12-b	@	9	133	1	2	18	163
12-c	@				1		1
12-d	@	4	129			12	145
12-h					1		1
13-a	@		18	8	167	81	274
13-b	@		8		7	1	16
13-d			4	1	7		12
13-e					6	2	8
13-f						2	2
14-a	@			92	239	10	341
14-b	@	13	4		15	3	35
14-c	@				3		3
14-d	@			3			3
14-e			16	6	1		23
14-f				5			5
15-a	@			3	55	11	69
16-a	@		15	243	66	13	337
16-c				5			5
16-d				8			8
17-d					1	1	2
17-e						1	1
18-a	@					1	1
18-c					5	3	8
18-d						4	4
18-e						1	1
19-b						1	2
19-c						165	165
20-a	@			169	13	5	187
21-a						1	1
30-a						21	21

(1) Structure types created by arranging the atoms with identical or similar geometrical positions. Such an arrangement always leads to a lower symmetry. In the rhombohedral system we found no such relations, unless we consider the examples given in Table 11 as belonging to this group.

(2) Structure types which have been "artificially" created by either a translation or a space group reduction. After translation or after combining two point sets, the structure types are the same and therefore incorrectly regarded as new structure types. Four examples are given in Table 12.

TABLE 11. Examples of structure types created by describing the arrangement of the atoms at lower symmetry sites

No.	Pearson symbol	Structure type	Space group number	Multiplicity and Wyckoff letter of point sets
108	<i>hR10</i>	FePSe ₃ -a	148	6c, 18f
109	<i>hR10</i>	FePSe ₃ -b	146	3a, 3a, 9b, 9b
177	<i>hR44</i>	Pd ₈ Sb ₃ -a	161	6a, 18b
178	<i>hR44</i>	Pd ₈ Sb ₃ -b	146	3a, 3b, 9b, 9b

TABLE 12. Examples of structure types created by either a translation of coordinates (by 0, 0, 1/2) or a space group reduction

No.	Pearson symbol	Structure type	Space group	Wyckoff positions
162	<i>hR5</i>	Ni ₃ S ₂	155	6c, 9e
				↓ ↓
164	<i>hR5</i>	Ni ₃ Se ₂	155	6c, 9d
112	<i>hR6</i>	Fe ₂ Tb	166	3b, 6c, 9e
				↓ ↓ ↓
124	<i>hR6</i>	GeRh ₃ Y ₂	166	3a, 6c, 9d
160	<i>hR7</i>	Ni ₃ Pb ₂ S ₂	166	3a, 3b, 6c, 9d
				↓ ↓ ↓ ↓
163	<i>hR7</i>	Ni ₃ S ₂ Sn ₂	166	3a, 3b, 6c, 9e
67	<i>hR19</i>	Be ₁₇ Nb ₂	166	6c, 6c, 9e, 18g, 18h
				↓ ↓ ↓ ↓ ↓
194	<i>hR19</i>	Th ₂ Zn ₁₇	166	6c, 6c, 9d, 18f, 18h

(3) Structure types which can have different space groups as well as different point sets but whose AETs are equal or similar. In our classification such structure types belong to the same coordination type. Some of these relations are well known from the literature, but with our approach we also trace new non-trivial relations.

These relations can easily be seen in our Tables 4-8. In Table 13 we give the observed relations between structure types for the two-, three-, four- and poly-environment groups.

TABLE 13. Structure types with equal AETs for the two-, three-, four- and poly-environment groups

Observed AETs (labels)	No.	Pearson symbol	Structure type
<i>Two-environment group</i>			
3#a + 4-a	121	<i>hR4</i>	GaSe
	2	<i>hR14</i>	Ag ₃ AsS ₂
	1	<i>hR24</i>	AgAsS ₂
3#a + 6-a	26	<i>hR25</i>	As ₄ Cu ₆ Hg ₃ S ₁₂
	30	<i>hR11</i>	As ₂ Ge ₃ Te ₆
	31	<i>hR13</i>	As ₂ Ge ₄ Te ₇
4-a + 6-a	175	<i>hR8</i>	P ₃ Sn
	21	<i>hR10</i>	Al ₂ O ₃
	140	<i>hR12</i>	Ir ₃ Se ₈
6-a + 6-b	87	<i>hR32</i>	Co ₂ Ge ₃ S ₃
	159	<i>hR4</i>	NbS ₂
	184	<i>hR6</i>	STi
6-b + 8-e	187	<i>hR8</i>	S ₁₂ Ti ₇
	185	<i>hR14</i>	S ₄ Ti ₃
	188	<i>hR14</i>	S ₁₄ Ti ₁₁
	186	<i>hR22</i>	S ₁₁ Ti ₈
	162	<i>hR5</i>	Ni ₃ S ₂
	164	<i>hR5</i>	Ni ₃ Se ₂
12-b + 12-d	193	<i>hR3</i>	Sm
	65	<i>hR12</i>	BaPb ₃
	120	<i>hR16</i>	Ga ₃ Pu
	20	<i>hR20</i>	Al ₃ Ho
12-a + 16-a	112	<i>hR6</i>	Fe ₂ Tb
	124	<i>hR6</i>	GeRh ₃ Y ₂
	6	<i>hR42</i>	AgMg ₅ Zn ₉
13-d + 14-e	7	<i>hR8</i>	AgNb ₄ S ₈
	8	<i>hR8</i>	AgS ₈ Ta ₄
13-b + 14-b	119	<i>hR14</i>	Ga ₄ Pd ₇ Zn ₃
	22	<i>hR26</i>	AlPd
<i>Three-environment group</i>			
3#a + 4-a + 6-a	138	<i>hR5</i>	In ₂ Se ₃
	135	<i>hR7</i>	In ₂ S ₄ Zn
	106	<i>hR9</i>	Fe ₂ Ga ₂ S ₅
	137	<i>hR9</i>	In ₂ S ₅ Zn ₂
	108	<i>hR10</i>	FePSe ₃ -a
	109	<i>hR10</i>	FePse ₃ -b
	182	<i>hR11</i>	Rh ₃ Se ₈
	79	<i>hR13</i>	C ₅ Ti ₈
	136	<i>hR14</i>	In ₂ S ₄ Zn
	13	<i>hR7</i>	Al ₄ C ₃
4-a + 5-a + 6-a	190	<i>hR22</i>	Sb ₃ Zn ₄
	176	<i>hR14</i>	Pd ₄ Pu ₃
12-a + 14-a + 16-a	180	<i>hR92</i>	Re ₂₅ Zr ₂₁
	66	<i>hR12</i>	Be ₃ Nb
12-a + 16-a + 20-a	85	<i>hR18</i>	Co ₇ Er ₂
	<i>Four-environment group</i>		
3#a + 4#b + 8-c + 12-a	160	<i>hR7</i>	Ni ₃ Pb ₂ S ₂
	163	<i>hR7</i>	Ni ₃ S ₂ Sn ₂
4-a + 4#b + 8-a + 10-a	82	<i>hR15</i>	CeMo ₆ S ₈
	147	<i>hR15</i>	Mo ₆ PbS ₈
	151	<i>hR44</i>	Mo ₉ S ₁₁ Tl ₂
12-a + 13-a + 14-a + 19-c	67	<i>hR19</i>	Be ₁₇ Nb ₂
	194	<i>hR19</i>	Th ₂ Zn ₁₇
12-a + 14-a + 15-a + 16-a	113	<i>hR13</i>	Fe ₇ W ₆
	84	<i>hR53</i>	Co ₅ Cr ₂ Mo ₃
<i>Poly-environment group</i>			
8-a + 10-c + 11-a + 12-a + 13-a	9	<i>hR44</i>	Al ₃ Au ₈
	177	<i>hR44</i>	Pd ₈ Sb ₃

A good example demonstrating the strength of our approach is found in the two-environment group by looking at the structures with the cubo-octahedron and the twinned cubo-octahedron, both having CN=12 and the labels 12-b and 12-d respectively. If we accept minor distortions from the ideal form due to properties of the constituent atoms, four structure types belong to this coordination type, namely 193 *hR3* Sm, 65 *hR12* BaPb₃, 120 *hR16* Ga₃Pu and 20 *hR20* Al₃Ho.

Special relations exist between the structure types consisting mainly of boron and it was very difficult to classify them with our approach. For example, in *hR12* B with two atoms in the asymmetrical unit as AETs, the monocapped (label 6-d) and the bicapped (label 7-d) pentagonal pyramid are realized. These AETs with pentagonal faces are typical of structures with boron and in our opinion this structure can much better be described as a structure consisting of cubic close-packed icosahedral B₁₂ clusters (see Figs. 8a and 8b). In contrast with our AETs, these clusters have no central atom.

In many papers these structure types are therefore treated as structure types containing clusters of boron atoms (see *e.g.* ref. 11).

A cubooctahedral boron cluster can be found in *cF52* B₁₂U, where we have the U atoms and the cubooctahedral B₁₂ clusters in a *cF8* ClNa type of lattice. In *cP7* B₆Ca we have octahedral boron clusters and the Ca atoms in a *cP2* ClCs type of lattice [11].

In some modifications of boron these icosahedral B₁₂ clusters are connected to each other by AETs which do have a central atom. For example, in *hR105* B these B₁₂ clusters are connected by an octahedron and in *tP50* B four of these B₁₂ clusters are connected by a tetrahedron.

The so-called Frank-Kasper structures are marked in our Tables 4-8 with the abbreviation F-K in the last column. Shoemaker and Shoemaker [12] give two rhombohedral structure types with Frank-Kasper coordination polyhedra. These structures are *hR13* Mo₆Co₇ and *hR53* Co₅₁Cr₁₈Mo₃₁. In addition to these two, we found that *hR6* Fe₂Tb, *hR6* GeRh₃Y₂, *hR42* AgMg₅Zn₉, *hR92* Re₂₅Zr₃₁, *hR13* Fe₇W₆ and *hR53* Co₅Cr₂Mo₃ are also Frank-Kasper structure types, the latter two being the same structure types as those named in ref. 12. The labels of the AETs observed in the F-K structure types are 12-a, 14-a, 15-a and 16-a.

6. Structure types with "improbable" interatomic distances

In ref. 1 we have extensively described the difficulties we encountered in the classification of structure types

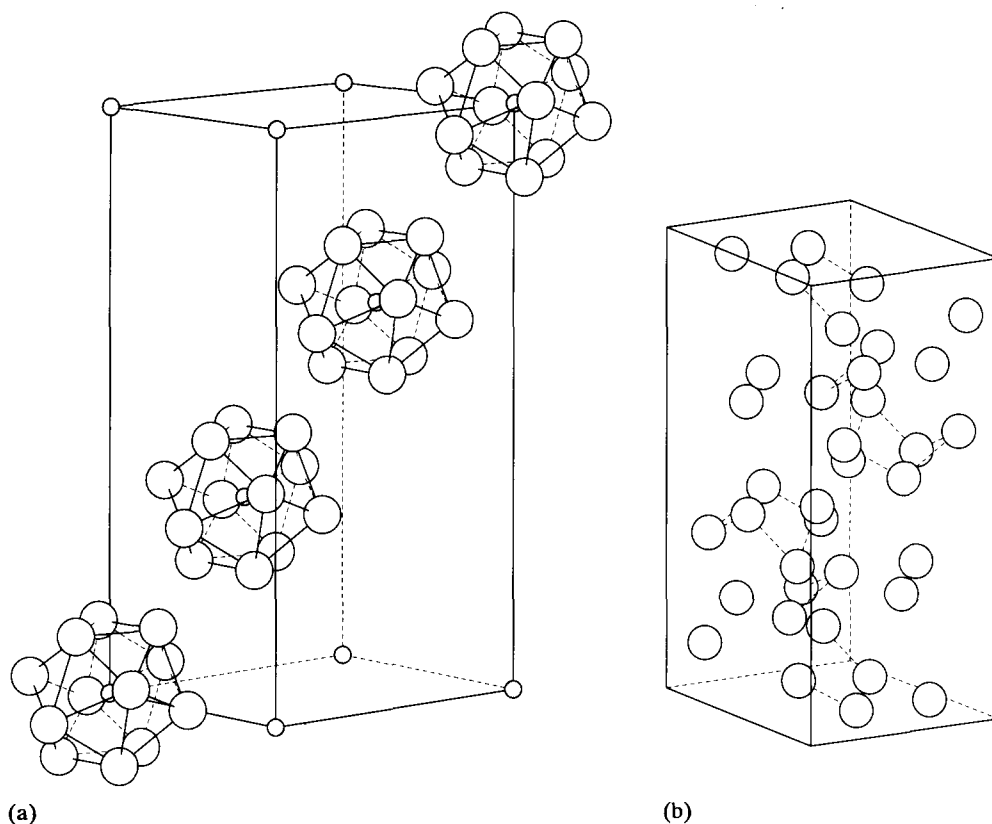


Fig. 8. The structure of *hR12 B* drawn (a) with and (b) without icosahedral B_{12} clusters; the centres of the B_{12} clusters are shaded in a.

with partly occupied point sets. Calculating interatomic distances in these structure types almost always results in these distances being too short. Also, although many of these structures have been published incorrectly, *e.g.* owing to printing errors, we have in ref. 1 extensively described how in some cases these inconsistencies can be removed.

We gave two possible solutions for these inconsistencies, both based on the fact that it is possible that these point sets are not statistically occupied. The first inconsistency can be removed when too short distances occur between atoms of the same point set and the occupation of this position is 0.5 or less. This means physically that this position cannot be occupied truly statistically and the short-range atomic arrangement probably has a lower symmetry. We call this an enantiomorphic principle, as explained in ref. 1, and it can be found in *e.g.* *hR8 Na₂S₃Sn*.

The second inconsistency exists when atoms are distributed over two point sets with fractional occupancies, say 0.75 and 0.25. In this situation it is not possible to find a simple enantiomorph. This ordering is only possible when an exclusion principle is in operation which prevents simultaneous occupation of both sides. This so-called exclusion principle can be observed in *e.g.* *hR20 Co₄Fe₄Th*.

In hydrogen- (deuterium-)containing structures we observed improbable interatomic distances, either too long (D–D) or too short (D–M). Owing to the variable size of the hydrogen (deuterium) atom, it is difficult to classify them. We observed that all the published hydrogen-containing structure types are derived from one of the three parent structures 66 *hR12 Be₃Nb*, 171 *hR17 P₂Pd₁₅* and 194 *hR19 Th₂Zn₁₇*.

Most of the structure types consisting mainly of boron have partly occupied point sets and therefore physically improbable interatomic distances. These problems and the aforementioned difficulties made us decide to exclude them all and we classified them as belonging to the filled-up type.

It is beyond the scope of this work to find the possible ordered structure types. In Table 14 we have listed 11 structure types in which such ordering could in principle occur and 17 filled-up types. We would like to stress that in these cases, where nature realises such ordering, the structure type represents an average situation of at least two different "pure" single phases. These structure types represent a rather "exotic" group of structures which have in general only one representative.

For the structure types given in Table 15, those with highly improbable short interatomic distances, the same holds, *i.e.* that they have only one representative.

TABLE 14. List of 28 excluded structure types with seemingly improbable interatomic distances (11) or so called filled-up structure types (17)

No.	Pearson symbol	Structure type	No. of representatives	Calculated shortest interatomic distance (nm)	
157	<i>hR8</i>	Na ₂ S ₃ Sn	1	S-S 0.0286	(1) See text
94	<i>hR14</i>	Cu ₅ FeS ₄	1	M3-M5 0.0306	(2) See text
3	<i>hR15</i>	Ag ₂ Cr ₇ S ₁₂	1	Ag1-Ag2 0.0505	(2)
150	<i>hR17</i>	Mo ₆ S ₈ Sn	1	Sn1-Sn2 0.0690	(2)
86	<i>hR20</i>	Co ₄ Fe ₄ Th	6	Th1-M1 0.1281	(2) See text
126	<i>hR20</i>	H ₂ HoNi ₃	1		(3) <i>hR12</i> Be ₃ Nb type
11	<i>hR21</i>	AlB ₄₀ C ₄	1		(3)
75	<i>hR22</i>	C ₂ Mn ₁₇ Pr ₂	20		(3) <i>hR19</i> Th ₂ Zn ₁₇ type
128	<i>hR23</i>	HP ₄ Pd ₃₀	1		(3) <i>hR17</i> P ₂ Pd ₁₅ type
103	<i>hR26</i>	Cu ₉ S ₅	1	Cu4-Cu5 0.0048	(2) See text
142	<i>hR26</i>	Li ₃ Mo ₉ S ₁₂	5	Li2-Li2 0.1152	(1)
146	<i>hR26</i>	Mo ₃ NiS ₄	11	Ni1-Ni2 0.1186	(2)
44	<i>hR29</i>	B ₁₉ C	1		(3)
64	<i>hR31</i>	Ba ₂ NbS ₅	2	Ba3-Ba3 0.0858	(1)
5	<i>hR46</i>	Ag ₈ GeTe ₆	1	Ag8-Ag12 0.0889	(2)
134	<i>hR73</i>	In ₄ SSe ₂ Te ₃	2	M3-Te1 0.0758	(2)
12	<i>hR113</i>	AlB ₅₂ Cu	1		(3)
52	<i>hR113</i>	B ₄₉ Fe	1		(3)
56	<i>hR115</i>	B ₂₃ Mn	1		(3)
61	<i>hR119</i>	B ₂₈ Sc	1		(3)
63	<i>hR119</i>	B ₅₁ Zr	1		(3)
62	<i>hR121</i>	B ₂₅ Zn	1		(3)
50	<i>hR133</i>	B ₂₃ Cu	1		(3)
51	<i>hR133</i>	B ₂₈ Cu	1		(3)
10	<i>hR137</i>	AlB ₃₁	1		(3)
39	<i>hR141</i>	B	1		(3)
58	<i>hR143</i>	B ₉₇ Ni ₂	1		(3)
54	<i>hR155</i>	B ₉₀ Ge	1		(3)

(1) Enantiomorphic principle; (2) exclusion principle; (3) filled-up structure.

TABLE 15. List of 23 excluded structure types with highly improbable interatomic distances (13), oxides (five), incomplete refinement (three) and p-element structures (two)

No.	Pearson symbol	Structure type	No. of representatives	Improbable short or long distance (nm), distance or other reason for exclusion
70	<i>hR2</i>	BiO	1	Oxide
125	<i>hR2</i>	GeTe	1	Ge-Te 0.5142
167	<i>hR2</i>	O ₂	1	No intermetallic
88	<i>hR5</i>	CrCuS ₂	5	Cu1-S1 0.1334
156	<i>hR7</i>	Na ₄ Pb ₂	1	Sodium not refined
55	<i>hR10</i>	B ₄ Li ₃	1	Li1-Li2 0.1046
53	<i>hR12</i>	B ₃ FeNd ₂	1	Boron not refined
98	<i>hR13</i>	CuMo ₃ S ₄	1	Cu1-Cu1 0.0998
127	<i>hR14</i>	H ₄ N ₂ Th	1	Hydrogen not refined
132	<i>hR16</i>	InMg ₃	1	In3-Mg2 0.1822
153	<i>hR16</i>	N ₂	1	No intermetallic
170	<i>hR16</i>	OZr ₃	1	Oxide
169	<i>hR19</i>	O ₁₂ Pr ₇	1	Oxide
14	<i>hR21</i>	Al ₆ C ₃ N ₂	2	See text
83	<i>hR21</i>	Ce ₇ O ₁₂	1	Oxide
189	<i>hR27</i>	STl ₂	1	S1-S2 0.0009
32	<i>hR28</i>	As ₄ Pb ₉ S ₁₅	1	S1-S2 0.1288, Pb2-S4 0.1329
168	<i>hR28</i>	O ₅ P ₂	1	Oxide
15	<i>hR29</i>	Al ₈ C ₃ N ₄	1	See text
74	<i>hR44</i>	C ₄ HgN ₄ Rb ₂	1	N2-C2 0.1109
78	<i>hR62</i>	CSi	1	Too long <i>c</i> axis
46	<i>hR96</i>	B ₈ Ce ₁₅ N ₂₅	1	Ce1-N4 0.2095
16	<i>hR168</i>	AlCa ₃ Cd ₁₇	1	Cd7-Cd38 0.1824 (see text)

In structure types with partly occupied point sets the Pearson symbol becomes questionable, especially in those structures where the full occupancy is prohibited by the geometry.

For some structure types we have tentatively redescribed the structures; we have replaced the partly occupied point set(s) by fully occupied point set(s) with a lower multiplicity.

An example of a redescribed structure type is given below and other examples are given in Table 16.

The structure type *hR20* Co₄Fe₄Th can be seen as a defect structure of the *hR19* Th₂Zn₁₇ structure type

in which the dumb-bell of the M1 atoms along the *c* axis is partly substituted by a Th atom at the origin. The opposite effect is frequently observed in the *hP6* CaCu₅ structure type [13]. In these compounds, *e.g.* LaNi₅, the rare earth atom at the origin is partly substituted by a dumb-bell of nickel atoms along the *c* axis and around the origin.

In the structure types 14 *hR21* Al₆C₃N₂ and 15 *hR29* Al₈C₃N₄ (their crystallographic data are given in the left half of Table 16) the atoms are created too close to each other. In fact, the description gives two atoms on each 6*c* position, *e.g.* in *hR14* Al₆C₃N₂ the Al1 atom

Old description						New description					
157 <i>hR8</i> Na ₂ S ₃ Sn Space group No. 166 <i>R3m</i>						90 <i>hR4</i> CrNaS ₂ type Space group No. 166 <i>R3m</i>					
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>
M	3 <i>a</i>	0	0	0	1	M	3 <i>a</i>	0	0	0	1
Na	3 <i>b</i>	0	0	$\frac{1}{2}$	1	Na	3 <i>b</i>	0	0	$\frac{1}{2}$	1
S	18 <i>h</i>	0.6915	0.3085	0.0730	0.33	S	6 <i>c</i>	$\frac{2}{3}$	$\frac{1}{3}$	0.0730	1

B, multiplicity and Wyckoff letter; *N*, occupancy.

TABLE 16. Crystallographic data of four examples of redescribed structure types

14 <i>hR21</i> Al ₆ C ₃ N ₂ Space group No. 166 <i>R3m</i>						14 <i>hR11</i> Al ₆ C ₃ N ₂ Space group No. 166 <i>R3m</i>						
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	
C1	3 <i>a</i>	0	0	0	1	C1	3 <i>a</i>	0	0	0	1	
Al1	6 <i>c</i>	0	0	0.6910	1	} →	Al1	6 <i>c</i>	0	0	0.6909	1
Al6	6 <i>c</i>	0	0	0.3092	1		Al2	6 <i>c</i>	0	0	0.0843	1
Al2	6 <i>c</i>	0	0	0.0850	1	} →	Al3	6 <i>c</i>	0	0	0.8079	1
Al5	6 <i>c</i>	0	0	0.9137	1		C2	6 <i>c</i>	0	0	0.1346	1
Al3	6 <i>c</i>	0	0	0.8069	1	} →	N2	6 <i>c</i>	0	0	0.7402	1
Al4	6 <i>c</i>	0	0	0.1911	1							
C2	6 <i>c</i>	0	0	0.1351	1							
C3	6 <i>c</i>	0	0	0.8641	1							
N1	6 <i>c</i>	0	0	0.7406	1							
N2	6 <i>c</i>	0	0	0.2597	1							
15 <i>hR29</i> Al ₈ C ₃ N ₄ Space group No. 166 <i>R3m</i>						15 <i>hR15</i> Al ₈ C ₃ N ₄ Space group No. 166 <i>R3m</i>						
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	
C1	3 <i>a</i>	0	0	0	1	C1	3 <i>a</i>	0	0	0	1	
Al1	6 <i>c</i>	0	0	0.6852	1	} →	Al1	6 <i>c</i>	0	0	0.6851	1
Al8	6 <i>c</i>	0	0	0.3250	1		Al2	6 <i>c</i>	0	0	0.0634	1
Al2	6 <i>c</i>	0	0	0.0633	1							
Al7	6 <i>c</i>	0	0	0.9365	1							

(continued)

TABLE 16. (continued)

15 <i>hR29</i> Al ₈ C ₃ N ₄ Space group No. 166 <i>R3m</i>						15 <i>hR15</i> Al ₈ C ₃ N ₄ Space group No. 166 <i>R3m</i>						
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	
Al3	6c	0	0	0.7752	1	} →	Al3	6c	0	0	0.7760	1
Al6	6c	0	0	0.2268	1		Al4	6c	0	0	0.1502	1
Al4	6c	0	0	0.1494	1	} →	Al4	6c	0	0	0.1502	1
Al5	6c	0	0	0.8522	1							
C2	6c	0	0	0.8112	1	} →	C2	6c	0	0	0.8117	1
C3	6c	0	0	0.1898	1							
N1	6c	0	0	0.7212	1	} →	N1	6c	0	0	0.7212	1
N4	6c	0	0	0.2788	1							
N2	6c	0	0	0.0993	1	} →	N2	6c	0	0	0.0992	1
N3	6c	0	0	0.9005	1							
94 <i>hR14</i> Cu ₅ FeS ₄ Space group No. 160 <i>R3m</i>						94 <i>hR5</i> Cu ₅ FeS ₄ Space group No. 160 <i>R3m</i>						
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	
M1	3a	0	0	0.000	1	} →	M1	3a	0	0	0.000	1
M2	3a	0	0	0.500	1		M2	3a	0	0	0.500	1
M3	3a	0	0	0.155	0.25	} →	M3	3a	0	0	0.150	1
M5	9b	0.973	0.027	0.142	0.25							
S1	3a	0	0	0.365	0.25	} →	M4	3a	0	0	0.356	1
M4	9b	0.027	0.973	0.378	0.25							
M6	9b	0.973	0.027	0.622	0.25	} →	M5	3a	0	0	0.630	1
S2	3a	0	0	0.635	0.25							
103 <i>hR26</i> Cu ₉ S ₅ Space group No. 166 <i>R3m</i>						103 <i>hR14</i> Cu ₉ S ₅ Space group No. 166 <i>R3m</i>						
Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	Atom	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>N</i>	
S1	3a	0	0	0	0.5	} →	C1	3a	0	0	0	0.5
Cu1	3b	0	0	0.500	0.5		Cu1	3b	0	0	0.500	0.5
Cu2	6c	0	0	0.060	0.5	} →	Cu2	6c	0	0	0.060	1
Cu3	6c	0	0	0.940	0.5							
Cu4	6c	0	0	0.133	0.5	} →	Cu3	6c	0	0	0.133	1
Cu5	6c	0	0	0.866	0.5							
Cu6	6c	0	0	0.250	0.5	} →	Cu4	6c	0	0	0.250	1
Cu7	6c	0	0	0.750	0.5							
Cu8	6c	0	0	0.350	0.5	} →	Cu5	6c	0	0	0.350	1
Cu9	6c	0	0	0.650	0.5							
S2	6c	0	0	0.200	0.5	} →	S2	6c	0	0	0.200	1
S3	6c	0	0	0.800	0.5							
S4	6c	0	0	0.400	0.5	} →	S3	6c	0	0	0.400	1
S5	6c	0	0	0.600	0.5							

B, multiplicity and Wyckoff letter; *N*, occupancy.

has the same atomic coordinates as the Al6 atom. This inconsistency can be removed if we redescribe the structures with six or eight atoms respectively in the asymmetrical unit (see right half of Table 16).

For this operation the originally given occupation numbers must be wrong of course, because in our description the Pearson symbol changes from *hR21* to *hR11* and from *hR29* to *hR15*.

A more or less similar effect is observed in 103 *hR26* Cu_9S_5 , although in this operation the occupation numbers change from 0.50 to 1.00 and the Pearson symbol to *hR14* (see Table 16).

It is of course unnecessary to emphasize that in all our redescribed structures we observed normal AETs after the redescription.

In the structure type *hR168* $\text{AlCa}_3\text{Cd}_{17}$ with 62 atoms in the asymmetrical unit we observed that the too short interatomic distances were always connected with the Cd38 atom (Cd38–Ca8 0.2452 nm, Cd38–Cd7 0.1824 nm, Cd38–Cd20 0.1891 nm). It seems that there is a printing error in the coordinates of this Cd38 atom.

7. Conclusions

Our analysis shows that in 4482 (71%) out of 6356 investigated AEs in rhombohedral systems nature prefers one of the 14 most symmetrical AETs shown in Fig. 2. Remarkably, these 14 AETs are equally often found in single-environment up to poly-environment groups, meaning that even in complex structures symmetrical AETs are preferred. In rhombohedral symmetry the geometrically simplest structure types are preferred, containing one, two, three or four AETs.

Most structure types with improbable interatomic distances can be classified according to the enantiomorphic or exclusion principle or are of the filled-up parent structure type.

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Appendix A

Number of times an AET is observed in the cubic structure types; an @ is added in the third column when the AET is also observed in the rhombohedral structure types

Old label	New label	Rhombohedral	Environment types					Total no. of structure types
			I	II	III	IV	Poly	
b	2#a	@			1	1		2
a	2#b	@			1			1
d	3#a	@		1	1	3		5
A	4-a	@	5	8	9	6	2	30

(continued)

Appendix A (continued)

Old label	New label	Rhombohedral	Environment types					Total no. of structure types
			I	II	III	IV	Poly	
g	4#b	@			2			2
e	4#c			1				1
B	5-a	@		3		2		5
h	5#b			1	1			2
C	6-a	@	5	9	9	4	2	34
1	6-b	@				2		2
j	6#c				1			1
2	7-a	@		1	2	2		5
D	7-b	@		1				1
3	7-c	@			1			1
E	8-a	@	1	9	3	1	1	15
4	8-b	@			1	1	1	3
F	9-a	@		3	4	4	3	14
7	9-b	@		1			2	3
6	9-c	@					1	1
H	10-a	@		4	2	2	2	10
9	10-b	@			1	1	5	7
G	10-c	@			2		3	5
8	10-d					1	1	2
10	10-e					1		1
I	11-a	@	1	1	4		1	7
J	11-b	@			2	1	2	5
11	11-c			1		1	2	4
12	11-d	@				1		1
K	12-a	@	1	11	12	12	12	48
L	12-b	@	5	1	6	1	2	15
N	12-c	@			1	4	6	11
M	12-d	@			1	2		3
15	12-e					1	2	3
13	12-f					1		1
14	12-g				1			1
O	13-a	@	1	1	6	3	9	20
P	13-b	@					2	2
16	13-c				1	1		2
Q	14-a	@		3	1	6	9	19
R	14-b	@	8		1		2	11
18	14-c	@		1			2	3
17	14-d	@			1	1		2
S	15-a	@				4	9	13
19	15-b						1	1
T	16-a	@		3	2	3	8	16
21	16-b					1		1
22	17-a				1	2		3
23	17-b					1	1	2
24	17-c					1		1
U	18-a	@			1	2	3	6
25	18-b						1	1
26	19-a						1	1
31	20-a	@					1	1
30	20-b				1			1
28	20-c				1			1
27	20-d				1			1
29	20-e			1				1
34	24-a			2				2
32	24-b				1			1
33	24-c			1				1
35	24-d				1			1

Appendix B

Number of times an AET is observed on a point set in the cubic structure types; an @ is added in the third column when the AET is also observed in the rhombohedral structure types

Old label	New label	Rhombohedral	Environment types					Total no. of point sets
			I	II	III	IV	Poly	
b	2#a	@			1	4		5
a	2#b	@			139			139
d	3#a	@		2	9	23		34
A	4-a	@	352	730	158	35	3	1278
g	4#b	@			29			29
e	4#c			2				2
B	5-a	@		121		25		146
h	5#b			1	8			9
C	6-a	@	1375	847	230	29	3	2484
1	6-b	@				3		3
j	6#c				1			1
2	7-a	@		6	25	26		57
D	7-b	@		36				36
3	7-c	@			1			1
E	8-a	@	8	527	31	158	4	728
4	8-b	@			6	6	77	89
F	9-a	@		53	47	66	5	171
7	9-b	@		1			14	15
6	9-c	@					1	1
H	10-a	@		347	22	6	2	377
9	10-b	@			68	2	18	88
G	10-c	@			3		7	10
8	10-d					4	1	5
10	10-e					3		3
I	11-a	@	2	1	42		4	49
J	11-b	@			8	13	3	24
11	11-c			6		2	2	10
12	11-d	@				2		2
K	12-a	@	2	1128	265	485	108	1988
L	12-b	@	1151	5	182	1	14	1353
N	12-c	@			4	80	15	99
M	12-d	@			3	6		9
15	12-e					4	2	6
13	12-f					2		2
14	12-g	@			3			3
O	13-a	@	90	3	114	165	113	485
P	13-b	@					61	61
16	13-c				4	2		6
Q	14-a	@		224	7	73	114	418
R	14-b	@	1879		4		100	1983
18	14-c	@		60			5	65
17	14-d	@			8	24		32
S	15-a	@				24	42	66
19	15-b						19	19
T	16-a	@		624	122	47	177	970
21	16-b					47		47
22	17-a				6	6		12
23	17-b					158	1	159
24	17-c					13		13
U	18-a	@			6	4	80	90
25	18-b						1	1
26	19-a						1	1

(continued)

Appendix B (continued)

Old label	New label	Rhombohedral	Environment types					Total no. of point sets
			I	II	III	IV	Poly	
31	20-a	@					13	13
30	20-b				41			41
28	20-c				16			16
27	20-d				1			1
29	20-e			6				6
34	24-a			20				20
32	24-b				68			68
33	24-c			54				54
35	24-d				16			16