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## Review

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# Atomic-environment classification of the cubic "intermetallic" structure types

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## Abstract

In this paper we give a complete description of the geometrical atomic environments found in the structure types of the cubic intermetallic compounds. Our analysis of 172 structure types which have been reported in the literature showed that 128 are geometrically possible, while the remaining 44 structure types have improbable interatomic distances. We have classified all point sets of these structure types in terms of the realized geometrical atomic environments and give rules for the analysis as well as the classification. In our systematic and comprehensive analysis of the cubic structure types we have verified all known relationships between these structure types, but the analysis also revealed new non-trivial relationships. In addition, we observed that 21 atomic environment types are strongly preferred. Out of 13 917 point sets investigated, 12 790 (92%) belong to one of those 21 atomic environment types. Of the 5521 compounds crystallizing into one of the 128 structure types, 46% belong to a single-environment group (structures in which all atoms have the same type of environment), 37% combine two environment types, 9% have three environments and the rest (8%) have four or more environments.

## 1. Introduction

For an interpretation of the physical and/or chemical properties of an intermetallic compound knowledge of its crystal structure is vital; for example, band-structure calculations are not possible without this knowledge. The structures given in the literature should therefore be correct.

Since a large number of structure types are compiled in *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, Vol. 1 [1], it is possible to look for rules governing the relations between them and the nature of these structures. Studying the atomic environments (AEs) as they are realized in the compounds known so far may give, in combination with the nature of the constituent atoms, a deeper insight into crystal chemistry and may eventually lead to the prediction of new structure types.

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We report on the investigation of the AEs of all structure types which are listed in ref. 1, after excluding all oxides and those with improbable interatomic distances, thus leaving 128 structure types representing 5521 compounds and 13 917 AEs (point sets). The AE analysis was performed after the transformation of all crystallographic data to the standard setting of the *International Tables for Crystallography*, Vol. A [2], and after comparing each entry with the original publication in order to prevent transcription errors.

In Table 1 the 172 structure types of the cubic intermetallic compounds are arranged alphabetically according to the formula and in Table 2 according to the Pearson symbol. For the convenience of the reader the structure types have been numbered, so a structure of interest can easily be traced throughout the tables.

The aim of our AE 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) What are the (as yet unknown) rules which relate the nature of the constituents of a compound to its crystal structure?

In Section 2 we present our method for defining an AE type (AET). Section 3 gives the observed AETs and with the aid of a number of examples we show that incorrect structure determinations lead to the realization of incorrect AEs. In Section 4 the results of the observed coordination types are briefly discussed and compared with results of other investigations.

Relations between the cubic structure types are given in Section 5 and some non-trivial relations are demonstrated with examples from other crystal symmetries. 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 AEs are correct.

## 2. Classification of crystal structures based on AEs

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 rather large number of different structure types (nearly 2000 types are listed in ref. 1, including the cubic structure types), which makes it almost impossible to see connections or even to detect identities. In addition, every year new structure types are being published, nowadays at a rate of about 60 per year.

The lattice symmetry and the space group of a compound are important for certain physical properties such as piezoelectricity and ferroelectricity, but for crystal chemistry they are less important. A minor change in the position of the atoms in a crystal structure can reduce its symmetry and

TABLE 1

Classical structure types arranged alphabetically

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 1 | cP48 | $Ag_3AuS_2$ | 4 | 2 |
| 2 | cI48 | $Ag_3AuTe_2$ | 3 | 3 |
| 3 | cI44 | $Ag_8Ca_3$ | 3 | 2 |
| 4 | cP64 | $Ag_6GaSe_6$ | 8 | Poly |
| 5 | cF220 | $Ag_9GaSe_6$ | 7 | e |
| 6 | cF312 | $Ag_8GeTe_6$ | 11 | e |
| 7 | cF336 | $Ag_8GeTe_6$ | 10 | e |
| 8 | cI52 | $Ag_2Hg_3$ | 4 | 2 |
| 9 | cI20 | $Ag_2S$ | 3 | e |
| 10 | cF260 | $Ag_5Te_3Tl$ | 7 | Poly |
| 11 | cP20 | $AlAu_4$ | 3 | 2 |
| 12 | cP84 | $Al_2BaS_4$ | 5 | 4 |
| 13 | cP24 | $Al_2CMo_3$ | 3 | 3 |
| 14 | cP72 | $Al_6CaTe_{10}$ | 5 | e |
| 15 | cF184 | $Al_{18}Cr_2Mg_3$ | 5 | 4 |
| 16 | cF84 | $Al_{13}Cr_4Si_4$ | 5 | Poly |
| 17 | cP52 | $Al_4Cu_9$ | 8 | 3 |
| 18 | cI276 | $Al_{19}Fe_4MnSi_2$ | 11 | e |
| 19 | cI96 | $AlLi_3N_2$ | 4 | 3 |
| 20 | cF12 | AlLiSi | 3 | 2 |
| 21 | cF1832 | $Al_3Mg_2$ | 23 | e |
| 22 | cF56 | $Al_2MgO_4$ | 3 | 2 |
| 23 | cI162 | $Al_6Mg_{11}Zn_{11}$ | 8 | 4 |
| 24 | cP138 | $Al_9Mn_2Si$ | 11 | Poly |
| 25 | cF56 | $Al_3Mo_8S_{16}$ | 5 | 2 |
| 26 | cP64 | AlSr | 8 | Poly |
| 27 | cP60 | $Al_7Sr_8$ | 7 | 4 |
| 28 | cF176 | $Al_{10}V$ | 4 | 4 |
| 29 | cI26 | $Al_{12}W$ | 2 | 2 |
| 30 | cP72 | $As_4Ba_4Si$ | 6 | 2 |
| 31 | cI32 | $As_3Co$ | 2 | 2 |
| 32 | cI64 | $AsCu_3$ | 2 | 1 |
| 33 | cP64 | $As_2Cu_{13}S_{17}SnV$ | 10 | 1 |
| 34 | cI54 | $As_7Hg_4S_{12}$ | 5 | e |
| 35 | cI46 | $As_8Hg_9S_{24}$ | 4 | e |
| 36 | cP28 | $AsNa_3S_3$ | 5 | 4 |
| 37 | cF24 | $AuBe_5$ | 3 | 2 |
| 38 | cP4 | $AuCu_3$ | 2 | 1 |
| 39 | cP76 | $Au_9In_4$ | 8 | e |
| 40 | cP40 | $Au_3NaSi$ | 3 | 3 |
| 41 | cI40 | $Au_3Sb_4Y_3$ | 3 | 3 |
| 42 | cP7 | $B_6Ca$ | 2 | 2 |
| 43 | cF1880 | $B_{66}Th$ | 14 | e |
| 44 | cF52 | $B_{12}U$ | 2 | 2 |
| 45 | cF1936 | $B_{66}Y$ | 14 | e |
| 46 | cF128 | $BaGe_2S_5$ | 4 | 3 |

(*continued*)

TABLE 1 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 47 | cP36 | $BaHg_{11}$ | 5 | Poly |
| 48 | cI160 | $Be_{17}Ru_3$ | 7 | 4 |
| 49 | cF88 | $Bi_4Cu_4Mn_3$ | 4 | 4 |
| 50 | cF72 | $BiCu_9S_6$ | 4 | e |
| 51 | cF16 | $BiF_3$ | 3 | 1 |
| 52 | cF88 | $Bi_4Mn_5Ni_2$ | 6 | Poly |
| 53 | cI120 | $Bi_4Rh$ | 2 | 2 |
| 54 | cF8 | C | 1 | 1 |
| 55 | cF116 | $C_6Cr_{23}$ | 5 | Poly |
| 56 | cP5 | $CFe_4$ | 2 | 1 |
| 57 | cF112 | $CFe_3W_3$ | 4 | 2 |
| 58 | cF36 | $C_2La$ | 2 | e |
| 59 | cF104 | $CMo_6Ni_6$ | 4 | 3 |
| 60 | cI40 | $C_3Pu_2$ | 2 | 2 |
| 61 | cP60 | $C_7V_8$ | 5 | 2 |
| 62 | cF12 | $CaF_2$ | 2 | 2 |
| 63 | cF32 | $Ca_7Ge$ | 3 | 1 |
| 64 | cF48 | $Ca_{33}Ge$ | 2 | e |
| 65 | cI32 | $Ca_3Hg$ | 3 | 1 |
| 66 | cP5 | $CaO_3Ti$ | 3 | 3 |
| 67 | cF1124 | $Cd_3Cu_4$ | 29 | Poly |
| 68 | cF1192 | $Cd_2Na$ | 17 | Poly |
| 69 | cP54 | $Cd_5Pt$ | 8 | e |
| 70 | cI392 | $Cd_5Pt$ | 18 | e |
| 71 | cF448 | $Cd_{45}Sm_{11}$ | 18 | Poly |
| 72 | cI184 | $Cd_6Y$ | 8 | e |
| 73 | cI176 | $Cd_6Yb$ | 8 | Poly |
| 74 | cF44 | $CeH_3$ | 3 | e |
| 75 | cP2 | ClCs | 2 | 1 |
| 76 | cF8 | ClNa | 2 | 1 |
| 77 | cF120 | CoMnSb | 5 | 3 |
| 78 | cF68 | $Co_9S_8$ | 4 | 4 |
| 79 | cI16 | CoU | 2 | 1 |
| 80 | cP26 | Cr | 3 | e |
| 81 | cF120 | $Cr_4H_7Zr_2$ | 3 | e |
| 82 | cF216 | $Cr_{21}La_6N_{23}$ | 8 | 1 |
| 83 | cP8 | $Cr_3Si$ | 2 | 2 |
| 84 | cF4 | Cu | 1 | 1 |
| 85 | cI96 | $CuFeS_2$ | 8 | 2 |
| 86 | cF256 | $Cu_5FeS_4$ | 5 | e |
| 87 | cF16 | $CuHg_2Ti$ | 4 | 1 |
| 88 | cI160 | CuLiSi | 7 | Poly |
| 89 | cF24 | $Cu_2Mg$ | 2 | 2 |
| 90 | cF76 | $Cu_4P_{10}Sn$ | 5 | e |
| 91 | cF196 | $Cu_7S_4$ | 2 | e |
| 92 | cI56 | $Cu_3S_3Sb$ | 4 | 3 |
| 93 | cF64 | $Cu_3S_4Sb$ | 3 | 3 |
| 94 | cI58 | $Cu_{12}S_{13}Sb_4$ | 5 | 4 |

(*continued*)

TABLE 1 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 95 | cP8 | $Cu_3S_4V$ | 3 | 3 |
| 96 | cF44 | $Cu_9Se_5$ | 3 | e |
| 97 | cI76 | $Cu_{15}Si_4$ | 3 | 3 |
| 98 | cF416 | $Cu_{41}Sn_{11}$ | 16 | 3 |
| 99 | cF28 | $Cu_3Te_2$ | 4 | e |
| 100 | cI52 | $Cu_5Zn_8$ | 4 | 3 |
| 101 | cF144 | $Dy_5Pd_2$ | 4 | e |
| 102 | cF436 | $Fe_{23}H_{16}Ho_6$ | 9 | e |
| 103 | cF244 | $Fe_{23}H_8Ho_6$ | 7 | e |
| 104 | cI34 | $Fe_4LaP_{12}$ | 3 | 3 |
| 105 | cP12 | $FeS_2$ | 2 | 2 |
| 106 | cF72 | $FeS_4Yb_2$ | 4 | e |
| 107 | cP8 | FeSi | 2 | 1 |
| 108 | cF408 | $Fe_{11}Zn_{39}$ | 14 | 4 |
| 109 | cI12 | Ga | 1 | 1 |
| 110 | cI168 | $Ga_4HfNi_2$ | 10 | e |
| 111 | cF52 | $GaMo_4S_8$ | 4 | 3 |
| 112 | cI112 | $Ga_4Ni_3$ | 3 | 3 |
| 113 | cP49 | $Ga_5Ni_8Zn_{36}$ | 8 | Poly |
| 114 | cI82 | $Gd_3Ni_8Sn_{16}$ | 5 | 4 |
| 115 | cI40 | $Ge_7Ir_3$ | 3 | 3 |
| 116 | cP64 | GeK | 4 | 3 |
| 117 | cI22 | $Ge_4Na_3Pt_4$ | 3 | 3 |
| 118 | cP14 | $HNb_3Sn$ | 3 | 2 |
| 119 | cF196 | $H_{16}Mn_{23}Th_6$ | 7 | e |
| 120 | cF200 | $H_{16}Mn_{23}Th_6$ | 8 | e |
| 121 | cF292 | $H_{30}Mn_{23}Th_6$ | 8 | e |
| 122 | cF152 | $H_8Mn_{23}Y_6$ | 7 | e |
| 123 | cF248 | $H_{18}Mn_{23}Y_6$ | 8 | e |
| 124 | cF344 | $H_{23}Mn_{23}Y_6$ | 9 | e |
| 125 | cF36 | $H_6RuSr_2$ | 3 | 3 |
| 126 | cP32 | $H_3U$ | 3 | 2 |
| 127 | cI14 | $HV_2$ | 2 | e |
| 128 | cF160 | $H_9V_4Zr_2$ | 5 | e |
| 129 | cI10 | $Hg_4Pt$ | 2 | 2 |
| 130 | cF128 | $In_3Li_{13}$ | 6 | 1 |
| 131 | cP72 | $In_5S_4$ | 5 | 2 |
| 132 | cF180 | $In_2Te_3$ | 7 | e |
| 133 | cF120 | $Ir_4Sc_{11}$ | 6 | Poly |
| 134 | cP54 | $K_4Si_{23}$ | 5 | 3 |
| 135 | cI58 | $La_6Ni_6P_{17}$ | 5 | 4 |
| 136 | cP96 | $Li_7MnN_4$ | 9 | 2 |
| 137 | cF432 | $Li_{22}Pb_5$ | 20 | 1 |
| 138 | cF396 | $Mg_6Pd$ | 14 | Poly |
| 139 | cF408 | $Mg_{44}Rh_7$ | 14 | 4 |
| 140 | cP39 | $Mg_2Zn_{11}$ | 6 | 4 |
| 141 | cP20 | Mn | 2 | 2 |
| 142 | cI58 | Mn | 4 | 3 |

(*continued*)

TABLE 1 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 143 | cI80 | $Mn_2O_3$ | 3 | 2 |
| 144 | cF116 | $Mn_{23}Th_6$ | 5 | 4 |
| 145 | cP8 | $Mo_3N_2$ | 4 | 1 |
| 146 | cP64 | $N_2$ | 2 | e |
| 147 | cI88 | $N_3U_2$ | 3 | 2 |
| 148 | cF160 | $NaSi_{14}$ | 5 | e |
| 149 | cF16 | NaTl | 2 | 1 |
| 150 | cF112 | $NaZn_{13}$ | 3 | 3 |
| 151 | cP12 | NiSSb | 3 | 2 |
| 152 | cF96 | $NiTi_2$ | 3 | 2 |
| 153 | cI28 | $P_4Th_3$ | 2 | 2 |
| 154 | cP64 | $Pb_4S_9Sb_2Sn$ | 5 | e |
| 155 | cI46 | $Pd_{16}S_7$ | 4 | 4 |
| 156 | cP64 | $Pd_{17}Se_{15}$ | 7 | 4 |
| 157 | cF104 | $Pd_{10}Te_3$ | 7 | 4 |
| 158 | cP1 | Po | 1 | 1 |
| 159 | cP40 | $Pr_3Rh_4Sn_{13}$ | 4 | 4 |
| 160 | cI34 | $Re_7Si_6U_4$ | 4 | 3 |
| 161 | cP140 | $Rh_{13}Sc_{57}$ | 13 | Poly |
| 162 | cI182 | $Rh_{14}Sc_{57}$ | 9 | e |
| 163 | cF116 | $Rh_6Sn_{18}Tb_5$ | 7 | Poly |
| 164 | cP252 | $RuZn_6$ | 14 | 3 |
| 165 | cI16 | $S_4Tl_3V$ | 3 | 3 |
| 166 | cP7 | $S_3U_4$ | 3 | 2 |
| 167 | cF8 | SZn | 2 | 1 |
| 168 | cF64 | $S_4Zr_3$ | 3 | 1 |
| 169 | cI54 | $Sb_2Tl_7$ | 4 | 1 |
| 170 | cI16 | Si | 1 | 1 |
| 171 | cP12 | $Si_2Sr$ | 2 | 2 |
| 172 | cI2 | W | 1 | 1 |

e, excluded because of improbable interatomic distances (see Tables 15 and 16).

may lead to a new mathematical description of structure (according to the rules given in ref. 2). The resulting deformation of the AE, however, may be negligible, so that the AET (defined below) does not change.

In our approach the structural classification is not only based on the mathematical description but we give information on the distinct AET present in the structure type, and we will show that a substantial reduction in the number of structure types is possible.

The aim of the AE concept described in the following is to define the AEs as clearly as possible, so that we will ultimately be able to group them into distinct AETs.

First, the maximum-gap rule is used: to define an AE we used the Brunner–Schwarzenbach method [3], where all interatomic distances between an atom and its neighbours are plotted in a histogram as shown in Fig. 1(a).

TABLE 2

Classical structure types arranged according to their Pearson symbol

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 84 | cF4 | Cu | 1 | 1 |
| 54 | cF8 | C | 1 | 1 |
| 76 | cF8 | ClNa | 2 | 1 |
| 167 | cF8 | SZn | 2 | 1 |
| 20 | cF12 | AlLiSi | 3 | 2 |
| 62 | cF12 | $CaF_2$ | 2 | 1 |
| 51 | cF16 | $BiF_3$ | 3 | 1 |
| 87 | cF16 | $CuHg_2Ti$ | 4 | 1 |
| 149 | cF16 | NaTl | 2 | 1 |
| 37 | cF24 | $AuBe_5$ | 3 | 2 |
| 89 | cF24 | $Cu_2Mg$ | 2 | 2 |
| 99 | cF28 | $Cu_3Te_2$ | 4 | e |
| 63 | cF32 | $Ca_7Ge$ | 3 | 1 |
| 58 | cF36 | $C_2La$ | 2 | e |
| 125 | cF36 | $H_6RuSr_2$ | 3 | 3 |
| 74 | cF44 | $CeH_3$ | 3 | e |
| 96 | cF44 | $Cu_9Se_5$ | 3 | e |
| 64 | cF48 | $Ca_{33}Ge$ | 2 | e |
| 44 | cF52 | $B_{12}U$ | 2 | 2 |
| 111 | cF52 | $GaMo_4S_8$ | 4 | 3 |
| 22 | cF56 | $Al_2MgO_4$ | 3 | 2 |
| 25 | cF56 | $Al_3Mo_8S_{16}$ | 5 | 2 |
| 93 | cF64 | $Cu_3S_4Sb$ | 3 | 3 |
| 168 | cF64 | $S_4Zr_3$ | 3 | 1 |
| 78 | cF68 | $Co_9S_8$ | 4 | 4 |
| 50 | cF72 | $BiCu_9S_6$ | 4 | e |
| 106 | cF72 | $FeS_4Yb_2$ | 4 | e |
| 90 | cF76 | $Cu_4P_{10}Sn$ | 5 | e |
| 16 | cF84 | $Al_{13}Cr_4Si_4$ | 5 | Poly |
| 49 | cF88 | $Bi_4Cu_4Mn_3$ | 4 | 4 |
| 52 | cF88 | $Bi_4Mn_5Ni_2$ | 6 | Poly |
| 152 | cF96 | $NiTi_2$ | 3 | 2 |
| 59 | cF104 | $CMo_6Ni_6$ | 4 | 3 |
| 157 | cF104 | $Pd_{10}Te_3$ | 7 | 4 |
| 57 | cF112 | $CFe_3W_3$ | 4 | 2 |
| 150 | cF112 | $NaZn_{13}$ | 3 | 3 |
| 55 | cF116 | $C_6Cr_{23}$ | 5 | Poly |
| 144 | cF116 | $Mn_{23}Th_6$ | 5 | 4 |
| 163 | cF116 | $Rh_6Sn_{18}Tb_5$ | 7 | Poly |
| 77 | cF120 | CoMnSb | 5 | 3 |
| 81 | cF120 | $Cr_4H_7Zr_2$ | 3 | e |
| 133 | cF120 | $Ir_4Sc_{11}$ | 6 | Poly |
| 46 | cF128 | $BaGe_2S_5$ | 4 | 3 |
| 130 | cF128 | $In_3Li_{13}$ | 6 | 1 |
| 101 | cF144 | $Dy_5Pd_2$ | 4 | e |
| 122 | cF152 | $H_8Mn_{23}Y_6$ | 7 | e |

(*continued*)

TABLE 2 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 128 | cF160 | $H_9V_4Zr_2$ | 5 | e |
| 148 | cF160 | $NaSi_{14}$ | 5 | e |
| 28 | cF176 | $Al_{10}V$ | 4 | 4 |
| 132 | cF180 | $In_2Te_3$ | 7 | e |
| 15 | cF184 | $Al_{18}Cr_2Mg_3$ | 5 | 4 |
| 91 | cF196 | $Cu_7S_4$ | 2 | e |
| 119 | cF196 | $H_{16}Mn_{23}Th_6$ | 7 | e |
| 120 | cF200 | $H_{16}Mn_{23}Th_6$ | 8 | e |
| 82 | cF216 | $Cr_{21}La_6N_{23}$ | 8 | 1 |
| 5 | cF220 | $Ag_9GaSe_6$ | 7 | e |
| 103 | cF244 | $Fe_{23}H_8Ho_6$ | 7 | e |
| 123 | cF248 | $H_{18}Mn_{23}Y_6$ | 8 | e |
| 86 | cF256 | $Cu_5FeS_4$ | 5 | e |
| 10 | cF260 | $Ag_5Te_3Tl$ | 7 | Poly |
| 121 | cF292 | $H_{30}Mn_{23}Th_6$ | 8 | e |
| 6 | cF312 | $Ag_8GeTe_6$ | 11 | e |
| 7 | cF336 | $Ag_8GeTe_6$ | 10 | e |
| 124 | cF344 | $H_{23}Mn_{23}Y_6$ | 9 | e |
| 138 | cF396 | $Mg_6Pd$ | 14 | Poly |
| 108 | cF408 | $Fe_{11}Zn_{39}$ | 14 | Poly |
| 139 | cF408 | $Mg_{44}Rh_7$ | 14 | 4 |
| 98 | cF416 | $Cu_{41}Sn_{11}$ | 16 | 3 |
| 137 | cF432 | $Li_{22}Pb_5$ | 20 | 1 |
| 102 | cF436 | $Fe_{23}H_{16}Ho_6$ | 9 | e |
| 71 | cF448 | $Cd_{45}Sm_{11}$ | 18 | Poly |
| 67 | cF1124 | $Cd_3Cu_4$ | 29 | Poly |
| 68 | cF1192 | $Cd_2Na$ | 17 | Poly |
| 21 | cF1832 | $Al_3Mg_2$ | 23 | e |
| 43 | cF1880 | $B_{66}Th$ | 14 | e |
| 45 | cF1936 | $B_{66}Y$ | 14 | e |
| 172 | cI2 | W | 1 | 1 |
| 129 | cI10 | $Hg_4Pt$ | 2 | 1 |
| 109 | cI12 | Ga | 1 | 1 |
| 127 | cI14 | $HV_2$ | 2 | e |
| 79 | cI16 | CoU | 2 | 1 |
| 165 | cI16 | $S_4Tl_3V$ | 3 | 3 |
| 170 | cI16 | Si | 1 | 1 |
| 9 | cI20 | $Ag_2S$ | 3 | e |
| 117 | cI22 | $Ge_4Na_3Pt_4$ | 3 | 3 |
| 29 | cI26 | $Al_{12}W$ | 2 | 2 |
| 153 | cI28 | $P_4Th_3$ | 2 | 2 |
| 31 | cI32 | $As_3Co$ | 2 | 2 |
| 65 | cI32 | $Ca_3Hg$ | 3 | 1 |
| 104 | cI34 | $Fe_4LaP_{12}$ | 3 | 3 |
| 160 | cI34 | $Re_7Si_6U_4$ | 4 | 3 |
| 41 | cI40 | $Au_3Sb_4Y_3$ | 3 | 3 |
| 60 | cI40 | $C_3Pu_2$ | 2 | 2 |

(*continued*)

TABLE 2 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 115 | cI40 | $Ge_7Ir_3$ | 3 | 3 |
| 3 | cI44 | $Ag_8Ca_3$ | 3 | 2 |
| 35 | cI46 | $As_8Hg_9S_{24}$ | 4 | e |
| 155 | cI46 | $Pd_{16}S_7$ | 4 | 4 |
| 2 | cI48 | $Ag_3AuTe_2$ | 3 | 3 |
| 8 | cI52 | $Ag_2Hg_3$ | 4 | 2 |
| 100 | cI52 | $Cu_5Zn_8$ | 4 | 3 |
| 34 | cI54 | $As_7Hg_4S_{12}$ | 5 | e |
| 169 | cI54 | $Sb_2Tl_7$ | 4 | 1 |
| 92 | cI56 | $Cu_3S_3Sb$ | 4 | 3 |
| 94 | cI58 | $Cu_{12}S_{13}Sb_4$ | 5 | 4 |
| 135 | cI58 | $La_6Ni_6P_{17}$ | 5 | 4 |
| 142 | cI58 | Mn | 4 | 3 |
| 32 | cI64 | $AsCu_3$ | 2 | 1 |
| 97 | cI76 | $Cu_{15}Si_4$ | 3 | 3 |
| 143 | cI80 | $Mn_2O_3$ | 3 | 2 |
| 114 | cI82 | $Gd_3Ni_8Sn_{16}$ | 5 | 4 |
| 147 | cI88 | $N_3U_2$ | 3 | 2 |
| 19 | cI96 | $AlLi_3N_2$ | 4 | 3 |
| 85 | cI96 | $CuFeS_2$ | 8 | 2 |
| 112 | cI112 | $Ga_4Ni_3$ | 3 | 3 |
| 53 | cI120 | $Bi_4Rh$ | 2 | 2 |
| 48 | cI160 | $Be_{17}Ru_3$ | 7 | 4 |
| 88 | cI160 | CuLiSi | 7 | Poly |
| 23 | cI162 | $Al_6Mg_{11}Zn_{11}$ | 8 | 4 |
| 110 | cI168 | $Ga_4HfNi_2$ | 10 | e |
| 73 | cI176 | $Cd_6Yb$ | 8 | Poly |
| 162 | cI182 | $Rh_{14}Sc_{57}$ | 9 | e |
| 72 | cI184 | $Cd_6Y$ | 8 | e |
| 18 | cI276 | $Al_{19}Fe_4MnSi_2$ | 11 | e |
| 70 | cI392 | $Cd_5Pt$ | 18 | e |
| 158 | cP1 | Po | 1 | 1 |
| 75 | cP2 | ClCs | 2 | 1 |
| 38 | cP4 | $AuCu_3$ | 2 | 1 |
| 56 | cP5 | $CFe_4$ | 2 | 1 |
| 66 | cP5 | $CaO_3Ti$ | 3 | 1 |
| 42 | cP7 | $B_6Ca$ | 2 | 2 |
| 166 | cP7 | $S_3U_4$ | 3 | 2 |
| 95 | cP8 | $Cu_3S_4V$ | 3 | 3 |
| 83 | cP8 | $Cr_3Si$ | 2 | 2 |
| 107 | cP8 | FeSi | 2 | 1 |
| 145 | cP8 | $Mo_3N_2$ | 4 | 1 |
| 105 | cP12 | $FeS_2$ | 2 | 2 |
| 151 | cP12 | NiSSb | 3 | 2 |
| 171 | cP12 | $Si_2Sr$ | 2 | 2 |
| 118 | cP14 | $HNb_3Sn$ | 3 | 2 |
| 11 | cP20 | $AlAu_4$ | 3 | 2 |
| 141 | cP20 | Mn | 2 | 2 |

(*continued*)

TABLE 2 (*continued*)

| No. | Pearson symbol | Structure type | No. of point sets | No. of AETs |
|---|---|---|---|---|
| 13 | cP24 | $Al_2CMo_3$ | 3 | 3 |
| 80 | cP26 | Cr | 3 | e |
| 36 | cP28 | $AsNa_3S_3$ | 5 | 4 |
| 126 | cP32 | $H_3U$ | 3 | 2 |
| 47 | cP36 | $BaHg_{11}$ | 5 | Poly |
| 140 | cP39 | $Mg_2Zn_{11}$ | 6 | 4 |
| 40 | cP40 | $Au_3NaSi$ | 3 | 3 |
| 159 | cP40 | $Pr_3Rh_4Sn_{13}$ | 4 | 4 |
| 1 | cP48 | $Ag_3AuS_2$ | 4 | 2 |
| 113 | cP49 | $Ga_5Ni_8Zn_{36}$ | 8 | Poly |
| 17 | cP52 | $Al_4Cu_9$ | 8 | 3 |
| 69 | cP54 | $Cd_5Pt$ | 8 | e |
| 134 | cP54 | $K_4Si_{23}$ | 5 | 3 |
| 27 | cP60 | $Al_7Sr_8$ | 7 | 4 |
| 61 | cP60 | $C_7V_8$ | 5 | 2 |
| 4 | cP64 | $Ag_6GaSe_6$ | 5 | 2 |
| 26 | cP64 | AlSr | 8 | Poly |
| 33 | cP64 | $As_2Cu_{13}S_{17}SnV$ | 10 | 1 |
| 116 | cP64 | GeK | 4 | 3 |
| 146 | cP64 | $N_2$ | 2 | e |
| 154 | cP64 | $Pb_4S_9Sb_2Sn$ | 5 | e |
| 156 | cP64 | $Pd_{17}Se_{15}$ | 7 | 4 |
| 14 | cP72 | $Al_6CaTe_{10}$ | 5 | e |
| 30 | cP72 | $As_4Ba_4Si$ | 6 | 2 |
| 131 | cP72 | $In_5S_4$ | 5 | 2 |
| 39 | cP76 | $Au_9In_4$ | 8 | e |
| 12 | cP84 | $Al_2BaS_4$ | 5 | 4 |
| 136 | cP96 | $Li_7MnN_4$ | 9 | 2 |
| 24 | cP138 | $Al_9Mn_2Si$ | 11 | Poly |
| 161 | cP140 | $Rh_{13}Sc_{57}$ | 13 | Poly |
| 164 | cP252 | $RuZn_6$ | 14 | 3 |

e, excluded because of improbable interatomic distances (see Tables 15 and 16).

The height of the bars is proportional to the number of neighbours $n$ and it is convenient to express all distances $d$ relative to the shortest distance $d_{min}$. In most cases a clear maximum gap is revealed, as can be seen in Fig. 1(a). The AE of Fig. 1(b) is constructed with the atoms to the left of this gap.

However, in a few cases this 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. An example of such an erroneous atomic environment, based on the maximum gap method, is given in Fig. 2. The AE constructed with the 6 + 12 atoms before the maximum gap in the next-neighbour histogram (Fig. 2(a)) is a cubo-octahedron (Fig. 2(b)) with the six first neighbours situated in the middle of the faces. For these incorrect environments we defined the following rule.

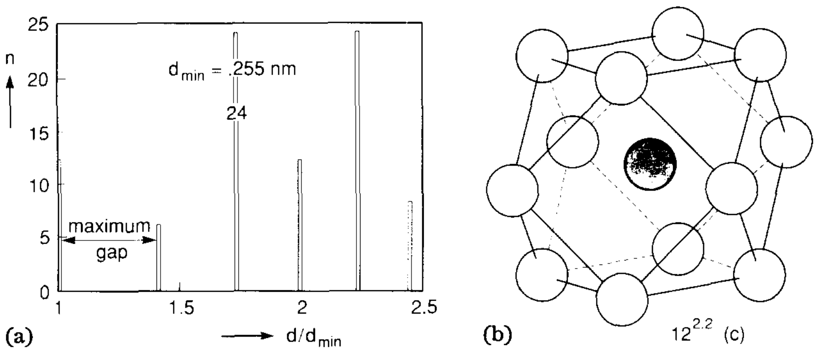


Fig. 1. (a) A typical example of a next-neighbour histogram and (b) the AE constructed with the atoms before the maximum gap in this histogram.

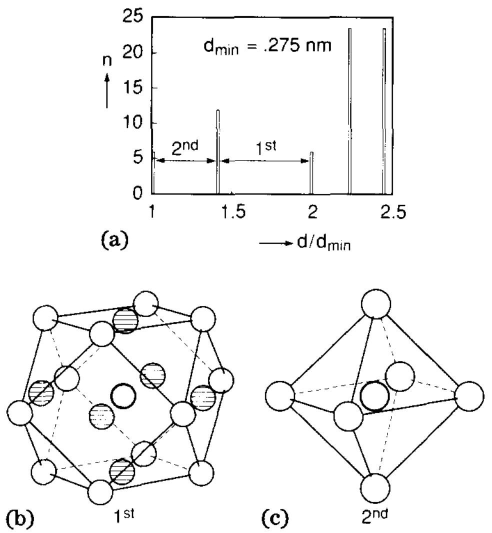


Fig. 2. (a) An example of a next-neighbour histogram with a "false" maximum gap, (b) the corresponding incorrect AET and (c) the correct AET.

The maximum-convex-volume 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. In Fig. 2(c) the correct AE, an octahedron, based on the maximum-convex-volume rule for the erroneous example given above is shown. Also, if no clear maximum gap was detectable, we used the maximum-convex-volume rule.

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. In the example given in Fig. 3 we have in the next-neighbour histogram two almost equal gaps and according to this practical rule we used in this structure type the atoms before the first gap, giving an AE in the form of an icosahedron with 12 coordinating atoms.

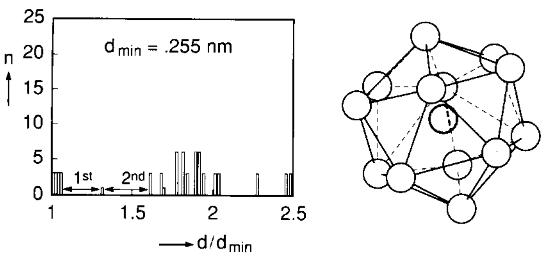
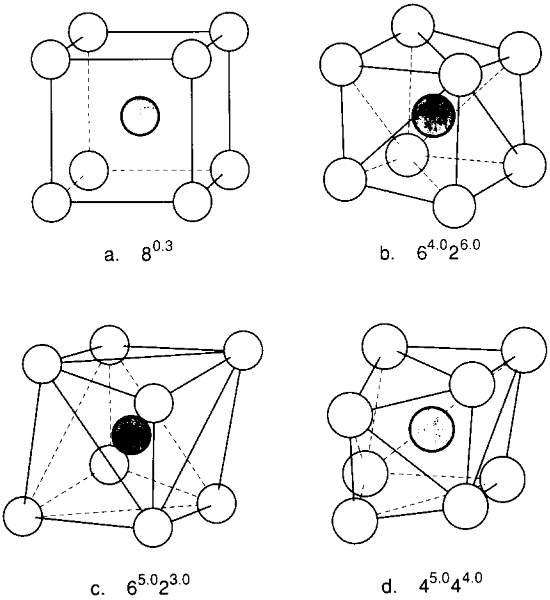


Fig. 3. An example of a next-neighbour histogram with two almost equal gaps, and the AET belonging to the first gap.



a. $8^{0.3}$

b. $6^{4.0}2^{6.0}$

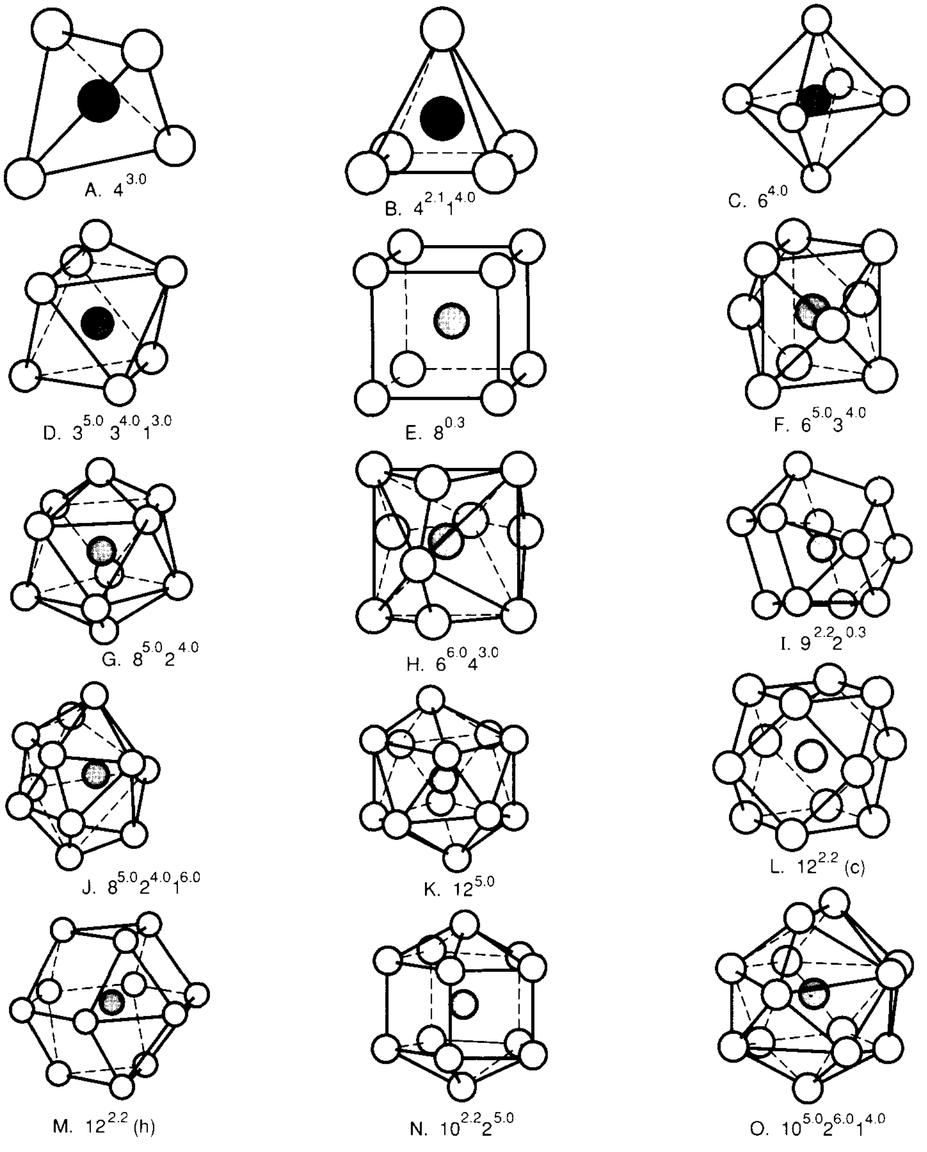
c. $6^{5.0}2^{3.0}$

d. $4^{5.0}4^{4.0}$

Fig. 4. Some distorted examples of the cube and their corresponding codes.

For constructing and displaying the AEs we used our own method, HISPOLY [4], by which the AEs are visualized as convex polyhedra with the surrounding atoms lying at the intersections of at least three faces. It is important to mention that our AETs are not isolated building units; crystal structures consist of interpenetrating AETs.

The AETs are characterized by using the codes as given in ref. 4, which are based on the number of triangles, squares, pentagons and hexagons that join each other in the different vertices (coordinating atoms). The code gives the number of equivalent vertices with the number of faces, in the above-mentioned sequence, as an exponent. For example, a quadratic pyramid has four corners adjoining two triangles, one square, no pentagon or hexagons, and one corner adjoining four triangles and nothing else. Its code, therefore, is $4^{2.1.0.0.}1^{4.0.0.0.}$ or, shorter, $4^{2.1}1^{4.0}$ with coordination number (CN) 5.



A. $4^{3.0}$ B. $4^{2.1}1^{4.0}$ C. $6^{4.0}$

D. $3^{5.0}3^{4.0}1^{3.0}$ E. $8^{0.3}$ F. $6^{5.0}3^{4.0}$

G. $8^{5.0}2^{4.0}$ H. $6^{6.0}4^{3.0}$ I. $9^{2.2}2^{0.3}$

J. $8^{5.0}2^{4.0}1^{6.0}$ K. $12^{5.0}$ L. $12^{2.2}$ (c)

M. $12^{2.2}$ (h) N. $10^{2.2}2^{5.0}$ O. $10^{5.0}2^{6.0}1^{4.0}$

Fig. 5. *(continued)*

However, this code is not unambiguous; it cannot differentiate between enantiomorphic AETs. Moreover, the code $12^{2.2}$ describes the cubic as well as the hexagonal AEs of the ideal close packings. Nor is the symmetry of the AET taken into account and therefore an ideal and an elongated cube have the same code. On the other hand, minor atomic shifts can create new edges and thus change the code of the AET. Since the bonding character is not changed seriously we assign the high-symmetry AET code to all related distorted AETs. In Fig. 4 some distorted cubes and their corresponding codes are illustrated.

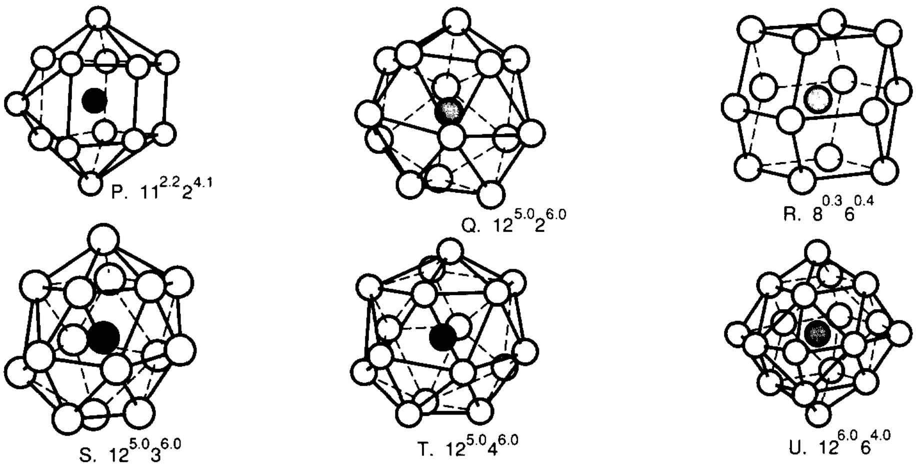


Fig. 5. The 21 most frequently occurring AETs with their codes and labels A–U.

Despite the above-mentioned drawback, the code remains very helpful due to the recognition of AET, *e.g.* the so-called Frank–Kasper polyhedra [5, 6] are easily recognized by their code. These four coordination polyhedra, with CNs of 12, 14, 15 and 16 respectively, are labelled K, Q, S and T in our list of most frequently occurring AETs (see Fig. 5.). The observed Frank–Kasper structure types are marked F–K under the heading remarks in Tables 3–7.

## 3. Observed AETs

Using the above-given rules we have analysed all 128 intermetallic structure types. Our approach leads to conventional AETs 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 128 structure types with 5521 compounds have 13 917 AEs (point sets). Of those AEs, 92% belong to one of the 21 most frequently occurring AETs shown in Fig. 5. AETs were added to this list when they were observed in different structure types.

The remaining normal AETs are shown in Fig. 6, and in Fig. 7 the IAETs are given. The 66 distinct high-symmetry AETs were derived from 292 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 shown in Fig. 4. In Figs. 5–7 these 66 AETs are listed together with their codes and labels (numbers), Fig. 5 with the labels A–U, Fig. 6 with the numbers 1–35 and Fig. 7 with the labels a–j.

TABLE 3

Structure types belonging to the single-environment group, ordered according to coordination types with increasing CNs

| No. | Pearson symbol | Structure type | No of point-sets | No. of compounds | Coordination number | Most frequently occurring Atomic Environment Types (AET) → label + coordination number | | | | | | | | | | | | | | | | | | | | | Rarely occurring AET | | Remarks |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | $A_4$ | $B_5$ | $C_6$ | $D_7$ | $E_8$ | $F_9$ | $G_{10}$ | $H_{10}$ | $I_{11}$ | $J_{11}$ | $K_{12}$ | $L_{12}$ | $M_{12}$ | $N_{12}$ | $O_{13}$ | $P_{13}$ | $Q_{14}$ | $R_{14}$ | $S_{15}$ | $T_{16}$ | $U_{18}$ | AET | IAET | |
| 54 | cF8 | C | 1 | 9 | 4 | X | | | | | | | | | | | | | | | | | | | | | | | |
| 170 | cI16 | Si | 1 | 1 | 4 | X | | | | | | | | | | | | | | | | | | | | | | | |
| 56 | cP5 | $CFe_4$ | 2 | 1 | 4 | X | | | | | | | | | | | | | | | | | | | | | | | |
| 167 | cF8 | SZn | 2 | 160 | 4 | X | | | | | | | | | | | | | | | | | | | | | | | |
| 33 | cP64 | $As_2Cu_{13}S_{17}SnV$ | 10 | 2 | 4 | X | | | | | | | | | | | | | | | | | | | | | | | |
| 158 | cP1 | Po | 1 | 9 | 6 | | | X | | | | | | | | | | | | | | | | | | | | | |
| 76 | cF8 | ClNa | 2 | 674 | 6 | | | X | | | | | | | | | | | | | | | | | | | | | |
| 168 | cF164 | $S_4Zr_3$ | 3 | 2 | 6 | | | X | | | | | | | | | | | | | | | | | | | | | |
| 145 | cP8 | $Mo_3N_2$ | 4 | 1 | 6 | | | X | | | | | | | | | | | | | | | | | | | | | |
| 82 | cF216 | $Cr_{21}La_6N_{23}$ | 8 | 1 | 6 | | | X | | | | | | | | | | | | | | | | | | | | | |
| 79 | cI16 | CoU | 2 | 1 | 11 | | | | | | | | | X | | | | | | | | | | | | | | | |
| 32 | cI64 | $AsCu_3$ | 2 | 1 | 12 | | | | | | | | | | | X | | | | | | | | | | | | | |
| 84 | cF4 | Cu | 1 | 369 | 12 | | | | | | | | | | | | X | | | | | | | | | | | | |
| 109 | cI12 | Ga | 1 | 1 | 12 | | | | | | | | | | | | X | | | | | | | | | | | | |
| 38 | cP4 | $AuCu_3$ | 2 | 386 | 12 | | | | | | | | | | | | X | | | | | | | | | | | | |
| 63 | cF32 | $Ca_7Ge$ | 3 | 2 | 12 | | | | | | | | | | | | X | | | | | | | | | | | | |
| 65 | cI32 | $Ca_3Hg$ | 3 | 1 | 12 | | | | | | | | | | | | X | | | | | | | | | | | | |
| 107 | cP8 | FeSi | 2 | 45 | 13 | | | | | | | | | | | | | | | X | | | | | | | | | |
| 172 | cI2 | W | 1 | 241 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 75 | cP2 | ClCs | 2 | 401 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 149 | cF16 | NaTl | 2 | 34 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 51 | cF16 | $BiF_3$ | 3 | 174 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 87 | cF16 | $CuHg_2Ti$ | 4 | 34 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 169 | cF54 | $Sb_2Tl_7$ | 4 | 1 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 130 | cF128 | $In_3Li_{13}$ | 6 | 1 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 137 | cF432 | $Li_{22}Pb_5$ | 20 | 5 | 14 | | | | | | | | | | | | | | | | | | X | | | | | | |
| 26 | structure types | | | 2557 compounds | | 352 | - | 1375 | - | - | | - | - | 2 | | 2 | 1151 | - | - | 90 | - | - | 1879 | - | - | | - | | 4851 point-sets |

In Fig. 8 the distribution frequency observed for the 21 most frequently occurring AETs in cubic structure types is plotted. It shows that the tetrahedron, octahedron, icosahedron, cubo-octahedron and the rhombic dodecahedron are strongly preferred for AETs.

Our results confirm the results of Villars *et al.* [7] who found in 147 intermetallic binary structure types (each of them having more than five representatives) almost the same AETs. It can be seen in Fig. 5 that nature seems to prefer highly symmetrical and beautiful AETs with even CNs. In Fig. 6, 35 less frequently occurring AETs are given; these are the AEs which are realized in just one or two structure types, each of them having only a few compounds.

At the moment it is not possible to decide whether these AETs are real or a consequence of the inaccuracy of the structure determination. This

TABLE 4

Structure types belonging to the two-environment group, ordered according to coordination types with increasing CNs

| | | | | | | Most frequently occurring Atomic Environment Types (AET) label + coordination number | | | | | | | | | | | | | | | | | | | | | Rarely occurring AET | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| No. | Pearson symbol | Structure type | No. of point-sets | No. of compounds | Coordination numbers | $A_4$ | $B_5$ | $C_6$ | $D_7$ | $E_8$ | $F_9$ | $G_{10}$ | $H_{10}$ | $I_{11}$ | $J_{11}$ | $K_{12}$ | $L_{12}$ | $M_{12}$ | $N_{12}$ | $O_{13}$ | $P_{13}$ | $Q_{14}$ | $R_{14}$ | $S_{15}$ | $T_{16}$ | $U_{18}$ | AET | IAET | Remarks |
| 131 | cP72 | $In_5S_4$ | 5 | 1 | 3/4 | X | | | | | | | | | | | | | | | | | | | | | | d (2) | |
| 31 | cI32 | $As_3Co$ | 2 | 19 | 4/6 | X | | X | | | | | | | | | | | | | | | | | | | | | |
| 105 | cP12 | $FeS_2$ | 2 | 152 | 4/6 | X | | X | | | | | | | | | | | | | | | | | | | | | |
| 22 | cF56 | $Al_2MgO_4$ | 3 | 218 | 4/6 | X | | X | | | | | | | | | | | | | | | | | | | | | |
| 151 | cP12 | NiSSb | 3 | 32 | 4/6 | X | | X | | | | | | | | | | | | | | | | | | | | | |
| 143 | cI80 | $Mn_2O_3$ | 3 | 42 | 4/6 | X | | X | | | | | | | | | | | | | | | | | | | | | |
| 166 | cP7 | $S_3U_4$ | 3 | 2 | 4/6 | | | X | | | | | | | | | | | | | | | | | | | | e (2) | |
| 25 | cF56 | $Al_3Mo_8S_{16}$ | 5 | 3 | 4/9 | X | | | | | X | | | | | | | | | | | | | | | | | | |
| 118 | cP14 | $H\,Nb_3Sn$ | 3 | 1 | 4/24 | X | | | | | | | | | | | | | | | | | | | | | 34 (1) | | |
| 61 | cP60 | $C_7V_8$ | 5 | 1 | 5/6 | | | X | | | | | | | | | | | | | | | | | | | | h (4) | |
| 60 | cI40 | $C_3Pu_2$ | 2 | 48 | 5/9 | | X | | | | X | | | | | | | | | | | | | | | | | | |
| 42 | cP7 | $B_6Ca$ | 2 | 54 | 5/24 | | X | | | | | | | | | | | | | | | | | | | | 33 (54) | | |
| 44 | cF52 | $B_{12}U$ | 2 | 19 | 5/24 | | X | | | | | | | | | | | | | | | | | | | | 34 (19) | | |
| 153 | cI28 | $P_4Th_3$ | 2 | 280 | 6/8 | | | X | | X | | | | | | | | | | | | | | | | | | | |
| 57 | cF112 | $C\,Fe_3W_3$ | 4 | 54 | 6/12 | | | X | | | | | | | | X | | | | | | | | | | | | | |
| 30 | cP72 | $As_4Ba_4Si$ | 6 | 9 | 7/8 | | | | X | X | | | | | | | | | | | | | | | | | | | |
| 171 | cP12 | $Si_2Sr$ | 2 | 6 | 7/20 | | | | | | | | | | | | | | | | | | | | | | 2 (6)<br>29 (6) | | |
| 129 | cI10 | $Hg_4Pt$ | 2 | 4 | 8/8 | | | | | X | | | | | | | | | | | | | | | | | 5 (4) | | |
| 147 | cI88 | $N_3U_2$ | 3 | 1 | 8/9 | | | | | X | X | | | | | | | | | | | | | | | | | | |
| 1 | cP48 | $Ag_3Au\,S_2$ | 4 | 1 | 8/9 | | | | | X | | | X | | | | | | | | | | | | | | 7 (1) | | |
| 62 | cF12 | $CaF_2$ | 2 | 112 | 8/10 | | | | | X | | | X | | | | | | | | | | | | | | | | |
| 20 | cF12 | Al Li Si | 3 | 104 | 8/10 | | | | | X | | | X | | | | | | | | | | | | | | | | |
| 85 | cI96 | $Cu\,Fe\,S_2$ | 8 | 1 | 8/10 | | | | | X | | | X | | | | | | | | | | | | | | | | |
| 136 | cP96 | $Li_7Mn\,N_4$ | 9 | 3 | 8/10 | | | | | X | | | X | | | | | | | | | | | | | | | | |
| 53 | cI120 | $Bi_4Rh$ | 2 | 1 | 8/11 | | | | | X | | | | X | | | | | | | | | | | | | | | |
| 29 | cI26 | $Al_{12}W$ | 2 | 6 | 11/12 | | | | | | | | | | | X | | | | | | | | | | | 11 (6) | | |
| 126 | cP32 | $H_3U$ | 3 | 5 | 12/12 | | | | | | | | | | | X | X | | | | | | | | | | | | |
| 8 | cI52 | $Ag_2Hg_3$ | 4 | 1 | 12/13 | | | | | | | | | | | X | | | | X | | | | | | | | | |
| 83 | cP8 | $Cr_3Si$ | 2 | 182 | 12/14 | | | | | | | | | | | X | | | | | | X | | | | | | | F - K |
| 141 | cP20 | Mn | 2 | 38 | 12/14 | | | | | | | | | | | X | | | | | | X | | | | | | | F - K |
| 11 | cP20 | $Al\,Au_4$ | 3 | 4 | 12/14 | | | | | | | | | | | X | | | | | | X | | | | | | | F - K |
| 152 | cF96 | $Ni\,Ti_2$ | 3 | 60 | 12/14 | | | | | | | | | | | X | | | | | | | | | | | 18 (60) | | |
| 89 | cF24 | $Cu_2Mg$ | 2 | 491 | 12/16 | | | | | | | | | | | X | | | | | | | | | X | | | | F - K |
| 37 | cF24 | $Au\,Be_5$ | 3 | 52 | 12/16 | | | | | | | | | | | X | | | | | | | | | X | | | | F - K |
| 3 | cI44 | $Ag_8Ca_3$ | 3 | 29 | 12/16 | | | | | | | | | | | X | | | | | | | | | | | 20 (29) | | |
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 35 structure types | | | | 2039 compounds | | 730 | 121 | 847 | 36 | 531 | 53 | – | 347 | 1 | – | 1128 | 5 | – | – | 3 | – | 224 | – | – | 595 | – | 186 | 5 | 4812 point-sets |

point is best demonstrated by comparing the AETs of compounds for which two structure determinations exist.

For example, in the two compounds for which the crystallographic data are given in Table 8, for eight atomic positions (out of 13) the AETs differ from one determination to the other, to the extent that even the CNs change.

TABLE 5

Structure types belonging to the three-environment group, ordered according to coordination types with increasing CNs

| | | | | | | Most frequently occurring Atomic Environment Types (AET) → label + coordination number | | | | | | | | | | | | | | | | | | | | | Rarely occurring AET | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| No | Pearson symbol | Structure type | No. of point sets | No. of compounds | Coordination numbers | $A_4$ | $B_5$ | $C_6$ | $D_7$ | $E_8$ | $F_9$ | $G_{10}$ | $H_{10}$ | $I_{11}$ | $J_{11}$ | $K_{12}$ | $L_{12}$ | $M_{12}$ | $N_{13}$ | $O_{13}$ | $P_{13}$ | $Q_{14}$ | $R_{14}$ | $S_{15}$ | $T_{16}$ | $U_{18}$ | AET | IAET | Remarks |
| 46 | cF128 | $BaGe_2S_5$ | 4 | 1 | 2/4/12 | X | | | | | | | | | | X | | | | | | | | | | | | b (1) | |
| 66 | cF5 | $CaO_3Ti$ | 3 | 139 | 2/6/12 | | | X | | | | | | | | | X | | | | | | | | | | | a (139) | |
| 111 | cF52 | $GaMo_4S_8$ | 4 | 9 | 3/4/9 | X | | | | | X | | | | | | | | | | | | | | | | | d (9) | |
| 165 | cI16 | $S_4Tl_3V$ | 3 | 8 | 4/4/14 | X | | | | | | | | | | | | | | | | | | | | | 17 (8) | g (8) | |
| 92 | cI56 | $Cu_3S_3Sb$ | 4 | 6 | 4/6/8 | X | | X | | | | | | | | | | | | | | | | | | | 4 (6) | | |
| 95 | cP8 | $Cu_3S_4V$ | 3 | 21 | 4/6/10 | | | X | | | | | X | | | | | | | | | | | | | | | g (21) | |
| 104 | cI34 | $Fe_4LaP_{12}$ | 3 | 41 | 4/6/20 | X | | X | | | | | | | | | | | | | | | | | | | 30 (41) | | |
| 115 | cI40 | $Ge_7Ir_3$ | 3 | 23 | 4/7/9 | X | | | | | X | | | | | | | | | | | | | | | | 2 (23) | | |
| 119 | cI96 | $AlLi_3N_2$ | 4 | 5 | 4/8/11 | X | | | | X | | | | | X | | | | | | | | | | | | | | |
| 117 | cI22 | $Ge_4Na_3Pt_4$ | 3 | 1 | 4/10/20 | X | | | | | | X | | | | | | | | | | | | | | | 27 (1) | | |
| 134 | cP54 | $K_4Si_{23}$ | 5 | 16 | 4/20/24 | X | | | | | | | | | | | | | | | | | | | | | 28 (16)<br>35 (16) | | |
| 125 | cF36 | $H_6RuSr_2$ | 3 | 8 | 5/6/12 | | | X | | | | | | | | | X | | | | | | | | | | | h (8) | |
| 93 | cF64 | $Cu_3S_4Sb$ | 3 | 1 | 6/7/10 | | | | | | | | X | | | | | | | | | | | | | | 3 (1) | j (1) | |
| 160 | cI34 | $Re_7Si_6U_4$ | 4 | 3 | 6/9/12 | | | X | | | X | | | | | | X | | | | | | | | | | | | |
| 59 | cF104 | $CMo_6Ni_6$ | 4 | 3 | 6/11/12 | | | X | | | | | | | X | X | | | | | | | | | | | | | |
| 13 | cP24 | $Al_2CMo_3$ | 3 | 7 | 6/12/14 | | | X | | | | | | | | X | | | | | | X | | | | | | | |
| 40 | cP40 | $Au_3NaSi$ | 3 | 2 | 6/13/16 | | | X | | | | | | | | | | | | X | | | | | X | | | | |
| 2 | cI48 | $Ag_3AuTe_2$ | 3 | 2 | 7/8/10 | | | | | | | X | | | | | | | | | | | | | | | 2 (2)<br>5 (2) | | |
| 41 | cI40 | $Au_3Sb_4Y_3$ | 3 | 19 | 8/12/12 | | | | | X | | | | | | X | X | | | | | | | | | | | | |
| 116 | cP64 | GeK | 4 | 6 | 9/17/18 | | | | | | X | | | | | | | | | | | | | | | X | 22 (6) | | |
| 150 | cF112 | $NaZn_{13}$ | 3 | 68 | 10/12/24 | | | | | | | | | | | X | | | | | | | | | | | 9 (68)<br>32 (68) | | |
| 164 | cP252 | $RuZn_6$ | 14 | 1 | 11/12/12 | | | | | | | | | X | | X | | | X | | | | | | | | | | |
| 100 | cI52 | $Cu_5Zn_8$ | 4 | 17 | 11/12/13 | | | | | | | | | X | | X | | | | X | | | | | | | | | |
| 17 | cP52 | $Al_4Cu_9$ | 8 | 9 | 11/12/13 | | | | | | | | | X | | X | | | | X | | | | | | | | | |
| 98 | cF416 | $Cu_{41}Sn_{11}$ | 16 | 2 | 11/12/13 | | | | | | | | | X | | X | | | | X | | | | | | | | | |
| 112 | cI112 | $Ga_4Ni_3$ | 3 | 3 | 12/12/12 | | | | | | | | | | | | X | X | | | | | | | | | 14 (3) | | |
| 97 | cI76 | $Cu_{15}Si_4$ | 3 | 7 | 12/12/13 | | | | | | | | | | | X | X | | | X | | | | | | | | | |
| 77 | cF120 | CoMnSb | 5 | 2 | 12/13/14 | | | | | | | | | | | X | | | | | | | X | | | | 16 (4) | | |
| 142 | cI58 | Mn | 4 | 60 | 12/13/16 | | | | | | | | | | | X | | | | X | | | | | X | | | | |
| 29 structure types | | | | 490 compounds | | 158 | – | 230 | – | 29 | 47 | 3 | 22 | 42 | 8 | 265 | 182 | 3 | 4 | 114 | – | 7 | 4 | – | 122 | 6 | 265 | 187 | 1698 point-sets |

Two of our less frequently occurring AETs stem from these compounds. The two compounds belong to the Al–Sr and the Cu–S–Sb system respectively. For the examples in the Al–Sr system, cP60 $Al_7Sr_8$ and cP64 AlSr, the structure determination of the latter is incorrect as stated by the author [8].

## 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.

TABLE 6

Structure types belonging to the four-environment group, ordered according to coordination types with increasing CNs

| No. | Pearson symbol | Structure type | No. of point-sets | No. of compounds | Coordination numbers | Most frequently occurring Atomic Environment Types (AET) → label + coordination number | | | | | | | | | | | | | | | | | | | | | Rarely occurring AET | | Remarks |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | $A_4$ | $B_5$ | $C_6$ | $D_7$ | $E_8$ | $F_9$ | $G_{10}$ | $H_{10}$ | $I_{11}$ | $J_{11}$ | $K_{12}$ | $L_{12}$ | $M_{12}$ | $N_{12}$ | $O_{13}$ | $P_{13}$ | $Q_{14}$ | $R_{14}$ | $S_{15}$ | $T_{16}$ | $U_{18}$ | AET | IAET | |
| 12 | cP84 | $Al_2BaS_4$ | 5 | 2 | 2/4/12/15 | X | | | | | | | | | | X | | | | | | | | X | | | | b (4) | |
| 94 | cI58 | $Cu_{12}S_{13}Sb_4$ | 5 | 6 | 3/4/6/8 | X | | X | | | | | | | | | | | | | | | | | | | 4 (6) | d (6) | |
| 135 | cI58 | $La_6Ni_6P_{17}$ | 5 | 2 | 3/4/6/13 | X | | X | | | | | | | | | | | | | | | | | | | 16 (2) | d (4) | |
| 36 | cP28 | $AsNa_3S_3$ | 4 | 13 | 3/7/11/17 | | | | | | | | | | X | | | | | | | | | | | | 2 (13)<br>24 (13) | d (13) | |
| 78 | cF68 | $Co_9S_8$ | 4 | 13 | 4/5/6/7 | X | X | X | | | | | | | | | | | | | | | | | | | 2 (13) | | |
| 156 | cP64 | $Pd_{17}Se_{15}$ | 7 | 4 | 4/5/6/9 | X | X | X | | | X | | | | | | | | | | | | | | | | | | |
| 155 | cI46 | $Pd_{16}S_7$ | 4 | 2 | 4/6/12/14 | X | | | | | | | | | | X | | | | | | X | | | | | 1 (1) | | |
| 114 | cI82 | $Gd_3Ni_8Sn_{16}$ | 5 | 1 | 6/12/14/18 | | | | | | | | | | | X | | | | | | X | | | | X | 1 (2) | | |
| 144 | cF116 | $Mn_{23}Th_6$ | 5 | 158 | 8/12/13/17 | | | | | X | | | | | | X | | | | X | | | | | | | 23 (158) | | |
| 159 | cP40 | $Pr_3Rh_4Sn_{13}$ | 4 | 47 | 9/12/14/16 | | | | | | X | | | | | | | | | | | X | | | X | | | | |
| 48 | cI160 | $Be_{17}Ru_3$ | 7 | 3 | 9/12/15/16 | | | | | | X | | | | | X | | | | | | X | | | | | 21 (47) | | |
| 27 | cP60 | $Al_7Sr_8$ | 7 | 3 | 9/15/17/18 | | | | | | X | | | | | | | | | | | | | X | | X | 22 (3) | | |
| 157 | cF104 | $Pd_{10}Te_3$ | 7 | 1 | 10/10/11/12 | | | | | | | | X | | | | X | | | | | | | | | | 9 (2)<br>12 (2) | | |
| 49 | cF88 | $Bi_4Cu_4Mn_3$ | 4 | 4 | 10/10/12/13 | | | | | | | | X | | | | | | | X | | | | | | | 8 (4)<br>15 (4) | | |
| 140 | cP39 | $Mg_2Zn_{11}$ | 6 | 3 | 10/12/13/17 | | | | | | | | | | | X | | | | X | | | | | | | 10 (3)<br>22 (3) | | |
| 28 | cF176 | $Al_{10}V$ | 4 | 2 | 11/12/12/12 | | | | | | | | | | | X | | | X | | | | | | | | 11 (2)<br>13 (2) | | |
| 108 | cF408 | $Fe_{11}Zn_{39}$ | 14 | 1 | 12/12/12/14 | | | | | | | | | | | X | | X | X | | | X | | | | | | | |
| 139 | cF408 | $Mg_{44}Rh_7$ | 14 | 5 | 12/12/12/14 | | | | | | | | | | | X | | X | X | | | X | | | | | | | |
| 15 | cI84 | $Al_{18}Cr_2Mg_3$ | 5 | 24 | 12/12/14/16 | | | | | | | | | | | X | | | X | | | | | | X | | 17 (24) | | |
| 23 | cI62 | $Al_6Mg_{11}Zn_{11}$ | 8 | 10 | 12/14/15/16 | | | | | | | | | | | X | | | | | | X | | X | X | | | | F - K |
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 20 | structure types | | | 304 | compounds | 35 | 25 | 29 | – | 158 | 66 | – | 6 | – | 13 | 485 | 1 | 6 | 80 | 165 | – | 73 | – | 24 | 47 | 4 | 304 | 27 | 1548 point-sets |

The 128 analysed structure types of Tables 1 and 2 can be divided into five groups according to the number of different AETs: (1) single-environment structures, *i.e.* where all atoms have the same AET (this group of 26 structure types containing 2557 representatives with a total of 4851 point sets can be subdivided into seven coordination types); (2) two-environment structures, *i.e.* with each of the atoms having one of the two AETs (this group of 35 structure types containing 2039 representatives with a total of 4812 point sets can be subdivided into 24 coordination types); (3) Three-environment structures, *i.e.* with each of the atoms having one of the three AETs (this group of 29 structure types containing 490 representatives with a total of 1698 point sets can be subdivided into 27 coordination types); (4) four-environment structures, *i.e.* with each of the atoms having one of the four AETs (this group of 20 structure types containing 304 representatives with a total of 1548 point sets can be subdivided into 19 coordination types); (5) polyenvironment structures combining more than four AETs (this group of 18 structure types (also 18 coordination types) contains 131 representatives with a total of 1008 point sets).

In Tables 3–7 the structures are arranged according to the number of environments from single environmental (Table 3) to polyenvironmental (Table

TABLE 7

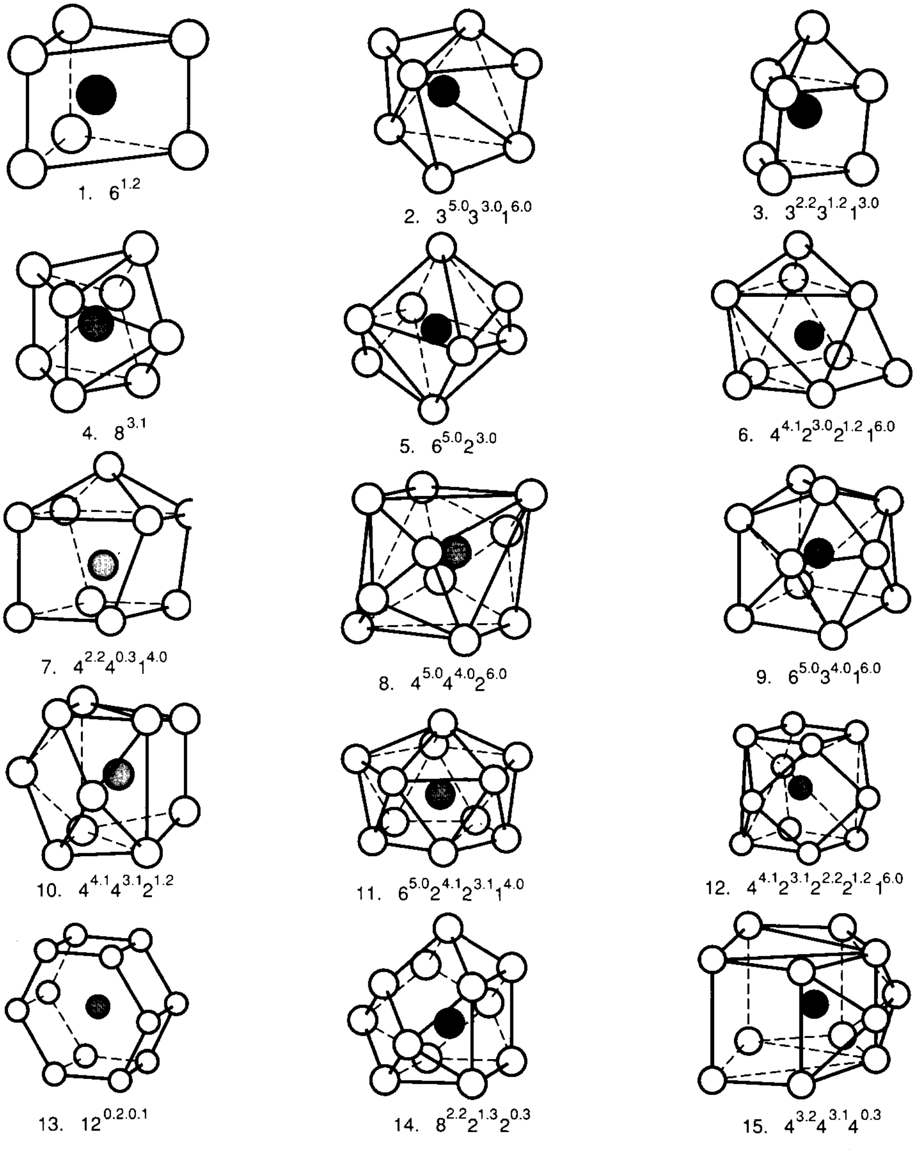
Structure types belonging to the polyenvironment group, ordered according to coordination types with increasing CNs

| No. | Pearson symbol | Structure type | No. of point-sets | No. of compounds | Coordination numbers | Most frequently occurring Atomic Environment Types (AET) → label + coordination number | | | | | | | | | | | | | | | | | | | | | Rarely occurring AET | | Remarks |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | $A_4$ | $B_5$ | $C_6$ | $D_7$ | $E_8$ | $F_9$ | $G_{10}$ | $H_{10}$ | $I_{11}$ | $J_{11}$ | $K_{12}$ | $L_{12}$ | $M_{12}$ | $N_{12}$ | $O_{13}$ | $P_{13}$ | $Q_{14}$ | $R_{14}$ | $S_{15}$ | $T_{16}$ | $U_{18}$ | AET | IAET | |
| 4 | cP64 | $Ag_9GaSe_6$ | 8 | 1 | 4/6/9/9/10 | X | | X | | | X | X | | | | | | | | | | | | | | | 7 (1) | | 5 AET |
| 16 | cF84 | $Al_{13}Cr_4Si_4$ | 5 | 1 | 4/10/12/12/12 | X | | | | | | | | | | X | | | X | | | | | | | | 9 (1)<br>15 (1) | | 5 AET |
| 52 | cF88 | $Bi_4Mn_5Ni_2$ | 6 | 1 | 6/10/10/10/12/12 | | | X | | | | | X | | | X | | | | | | | | | | | 8 (10)<br>9 (1)<br>15 (1) | | 6 AET |
| 133 | cF120 | $Ir_4Sc_6$ | 6 | 4 | 8/12/13/13/14 | | | | | X | | | | | | X | | | | X | X | | X | | | | 4 | | 5 AET |
| 55 | cF116 | $C_6Cr_{23}$ | 5 | 77 | 8/13/14/16/18 | | | | | | | | | | | | | | | X | | X | | | X | X | **4 (77)** | | 5 AET |
| 47 | cP36 | $BaHg_{11}$ | 5 | 13 | 9/10/12/15/20 | | | | | | | | | | | | X | | | | | | | X | | | 7 (13)<br>9 (13)<br>31 (13) | | 5 AET |
| 26 | cP64 | ALSr | 8 | 1 | 9/10/16/18/19 | | | | | | X | X | | | | | | | | | | | | | X | X | 26 (9) | | 5 AET |
| 10 | cF260 | $Ag_5Te_3Tl$ | 7 | 1 | 9/11/12/13 13/14/17 | | | | | | | | | | | | X | | X | X | | | X | | | | 6 (1)<br>11 (1)<br>23 (1) | | 7 AET |
| 163 | cF116 | $Rh_6Sn_{18}Tb_5$ | 7 | 2 | 9/13/14/16/18 | | | | | | X | | | | | | | | | X | | X | | | X | X | | | 5 AET |
| 113 | cP49 | $Ga_5Ni_8Zn_{36}$ | 8 | 1 | 10/10/12/13/15 | | | | | | | | X | | | X | | | | X | | | | X | | | 9 (1) | | 5 AET |
| 138 | cF396 | $Mg_6Pd$ | 14 | 3 | 10/12/12/13/14/14/16 | | | | | | | X | | | | X | | | X | X | | X | | | X | | 18 (1) | | 7 AET |
| 73 | cI176 | $Cd_6Yb$ | 8 | 1 | 10/12/13/15/18 | | | | | | | | | | | X | | | | X | | | | X | | | 9 (2)<br>25 (1) | | 5 AET |
| 24 | cP138 | $Al_9Mn_2Si$ | 11 | 2 | 11/11/12/12/13/14/15 | | | | | | | | | X | X | X | | | X | X | | X | | X | | | | | 7 AET |
| 161 | cP140 | $Rh_{13}Sc_{53}$ | 13 | 1 | 11/12/12/13/14/15 | | | | | | | | | | X | X | | | X | X | | X | | X | | | | | 6 AET |
| 88 | cI160 | CuLiSi | 7 | 1 | 11/12/14/15/16 | | | | | | | | | | | X | | | | | | X | | X | X | | 11 (1) | | 5 AET |
| 67 | cF1124 | $Cd_3Cu_4$ | 29 | 1 | 12/12/14/14/15/16 | | | | | | | | | | | X | | | X | | | X | | X | X | | 18 (2) | | 6 AET |
| 71 | cF448 | $Cd_{45}Sm_{11}$ | 18 | 19 | 12/13/14/14/15/15/16 | | | | | | | | | | | X | | | | | X | X | X | X | X | | 19 (19) | | 7 AET |
| 68 | cF1192 | $Cd_2Na$ | 17 | 1 | 12/13/14/15/16 | | | | | | | | | | | X | | | | X | | X | | X | X | | | | 5 AET |
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 18 | structure types | | | 131 | compounds | 3 | – | 3 | – | 4 | 5 | 7 | 2 | 4 | 3 | 108 | 14 | – | 15 | 113 | 61 | 114 | 100 | 42 | 177 | 80 | 153 | – | 1008 point-sets |

7). The labels for the AETs (A–U, 1–35, a–j) are the keys to the AETs and IAETs given in Figs. 5–7.

In the single-environment group we observed seven coordination types, giving a reduction of 73% compared with the 26 structure types. In the other environment groups the reduction is less pronounced; two-environment group, 32%; three-environment group, 7%; four-environment group, 5%; and no reduction in the polyenvironment group.

By combining our results for the single-environment group with the results of ref. 7, in which 5500 binary compounds crystallizing not only in cubic symmetry are analysed, the number of structure types increases to 50, but the number of coordination types only to 12. Therefore it can be expected that, upon a complete analysis of all crystal systems, the number of coordination types will be significantly lower than the number of structure types, especially since we know that 92% of all compounds crystallize within the first three groups, with one, two or three AETs respectively, as is demonstrated in Fig. 9.



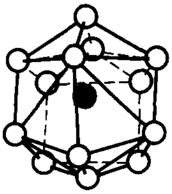
1. $6^{1.2}$
2. $3^{5.0}3^{3.0}1^{6.0}$
3. $3^{2.2}3^{1.2}1^{3.0}$
4. $8^{3.1}$
5. $6^{5.0}2^{3.0}$
6. $4^{4.1}2^{3.0}2^{1.2}1^{6.0}$
7. $4^{2.2}4^{0.3}1^{4.0}$
8. $4^{5.0}4^{4.0}2^{6.0}$
9. $6^{5.0}3^{4.0}1^{6.0}$
10. $4^{4.1}4^{3.1}2^{1.2}$
11. $6^{5.0}2^{4.1}2^{3.1}1^{4.0}$
12. $4^{4.1}2^{3.1}2^{2.2}2^{1.2}1^{6.0}$
13. $12^{0.2.0.1}$
14. $8^{2.2}2^{1.3}2^{0.3}$
15. $4^{3.2}4^{3.1}4^{0.3}$

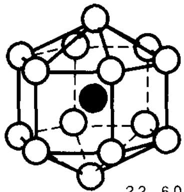
Fig. 6. *(continued)*

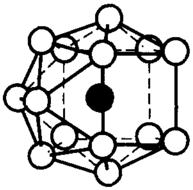
## 5. Related structure types

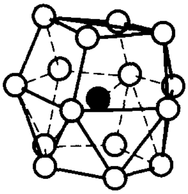
One of the main advantages of our analysis method is that it is easy to find relations between structures, which enable a differentiation to be made between three types of structural relations.

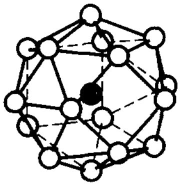
(a) Structure types created by arranging the atoms with identical or similar geometrical positions of the atoms always lead to a lower symmetry. In the cubic system we found five such relations which are given in Table 9.

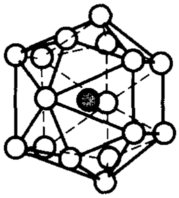

16. $4^{4.1}4^{2.2}2^{5.0}2^{4.0}1^{6.0}$

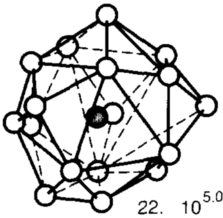

17. $12^{2.2}2^{6.0}$

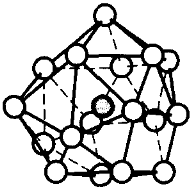

18. $6^{5.0}4^{4.1}4^{2.2}$

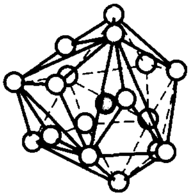

19. $3^{2.2}2^{4.1}\ 2^{4.0.1.0}2^{3.1}$
$2^{3.0.1.0}2^{1.2}1^{4.2}1^{2.0.1.0}$

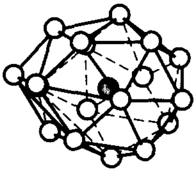

20. $8^{5.0}8^{4.1}$

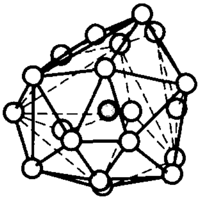

21. $8^{4.1}4^{6.0}4^{4.0}$

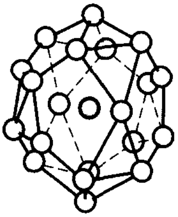

22. $10^{5.0}4^{4.1}3^{6.0}$

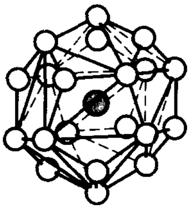

23. $8^{4.1}4^{5.0}4^{2.2}1^{0.4}$

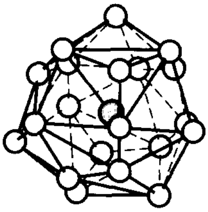

24. $7^{6.0}4^{3.0}3^{8.0}3^{4.0}$


25. $8^{5.0}5^{6.0}4^{4.1}1^{4.0}$


26. $9^{5.0}6^{7.0}3^{3.0}1^{6.0}$


27. $16^{2.0.2.0}4^{1.0.2.0}$


28. $12^{7.0}8^{3.0}$


29. $12^{6.0}6^{5.0}2^{3.0}$

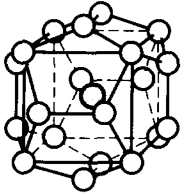

30. $12^{1.2}8^{3.3}$

Fig. 6. (*continued*)

(b) Structure types may be "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; three examples are given in Tables 10 and 11.

(c) Structure types can have different space groups as well as different point sets, but their AETs are equal or similar. In our classification such structure types belong to the same coordination type. Some of these relations

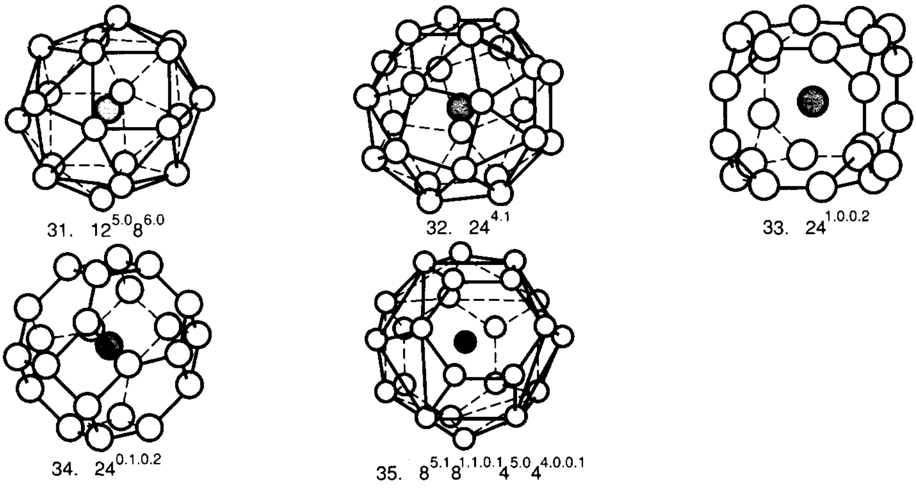


Fig. 6. The 35 least frequently occurring AETs with their codes and numbers 1–35.

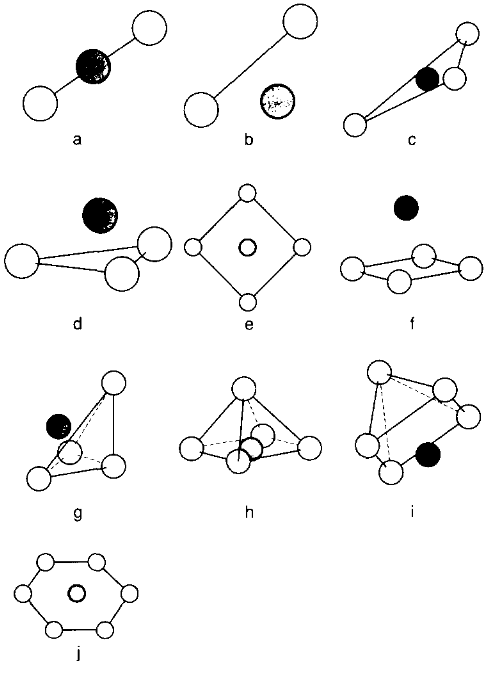


Fig. 7. The ten IAETs with their CNs and labels a–j.

are well known from the literature, but with our approach we also trace the new non-trivial relations.

A good example demonstrating the strength of our approach can be seen in the single-environment group, looking at the rhombic dodecahedron coordination type (CN = 14; code, $8^{0.3}6^{0.4}$; label, R). If we accept minor distortions from the ideal form, due to properties of the constituent atoms,

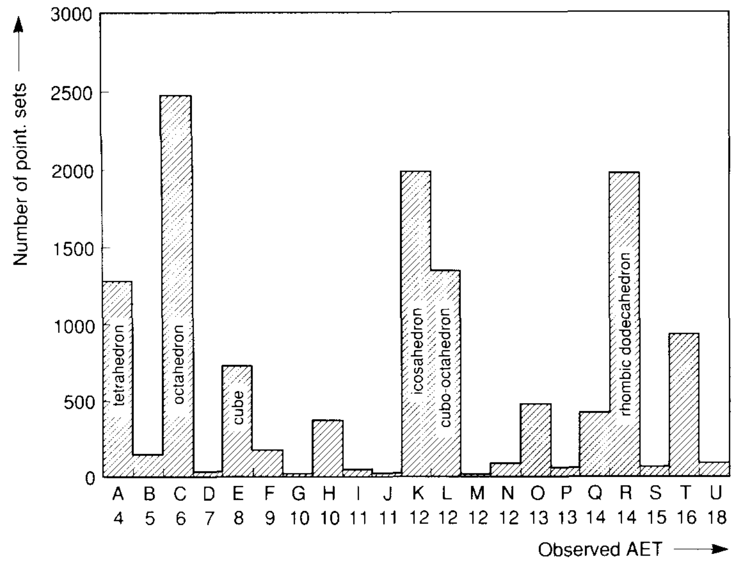


Fig. 8. A frequency plot of the 21 most frequently occurring AETs.

eight structure types belong to this coordination type. Five of them are quite trivial; 172 cI2 W, 75 cP2 ClCs, 149 cF16 NaTl, 51 cF16 $BiF_3$ and 87 cF16 $CuHg_2Ti$. The other three belonging to this coordination type, 169 cI54 $Sb_2Tl_7$, 130 cF128 $In_3Li_{13}$ and 137 cF432 $Li_{22}Pb_5$, are less obvious. In the last structure type we have 20 point sets, all having slightly distorted rhombic dodecahedrons as an AET. We observe that such relations are independent of the Bravais type (cF or cI or cP) and independent of the number of atoms in the unit cell (2–432). From the work done in ref. 7 we know that tP2 HgMn, tP4 CuTi and tI6 $MoSi_2$ also belong to this coordination type, showing us that the relations may even be independent of the crystal system. These relations can easily be seen in our Tables 3–7. In Table 12 we give some new non-trivial relations between structure types for the two-, three- and four-atom environment groups.

Some good examples of relations between structure types are given in refs. 9 and 10, both reporting the overlooked rhombohedral symmetry in crystal structures published with monoclinic *c*-centred lattices. In the paper by Cenzual *et al.* [10] mathematical rules are given for transformation of the monoclinic setting into the rhombohedral description for more examples. Although these structures do not belong to the cubic structure types, the structures described in ref. 9 are good examples to demonstrate our method. The structures described in this paper (their crystallographic data are given in Table 13) are mC32 $RbGa_7$ and hR16 $RbGa_7$, and Van Vucht has shown that the rhombohedral description he gives is identical to the monoclinic description by Belin [11].

Our analysis showed that the realized AEs are the same for both rubidium atoms with CN = 21, monoclinic (mC) as well as rhombohedral setting (hR),

TABLE 8

Crystallographic data of "identical" structure determinations in the systems Al–Sr and Cu–S–Sb

| No. | Pearson symbol | Structure type | Space group | $a$ (nm) | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ | $N^{(2)}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | cP60 | $Al_7Sr_8$ | $P2_13^a$ | 1.2753 | Al1 | 4a | 0.430 | 0.430 | 0.430 | 1 |
| | | | | | Sr1 | 4a | 0.815 | 0.815 | 0.815 | 1 |
| | | | | | Sr2 | 4a | 0.185 | 0.185 | 0.185 | 1 |
| | | | | | Al2 | 12b | 0.755 | 0.194 | 0.575 | 1 |
| | | | | | Al3 | 12b | 0.750 | 0.685 | 0.580 | 1 |
| | | | | | Sr3 | 12b | 0.806 | 0.559 | 0.004 | 1 |
| | | | | | Sr4 | 12b | 0.520 | 0.700 | 0.939 | 1 |
| 26 | cI64 | AlSr | $P2_13^a$ | 1.2753 | Al1 | 4a | 0.424 | 0.424 | 0.424 | 1 |
| | | | | | Sr1 | 4a | 0.814 | 0.814 | 0.814 | 1 |
| | | | | | Sr2 | 4a | 0.181 | 0.181 | 0.181 | 1 |
| | | | | | Al2 | 12b | 0.759 | 0.189 | 0.574 | 1 |
| | | | | | Al3 | 12b | 0.748 | 0.679 | 0.584 | 1 |
| | | | | | Sr3 | 12b | 0.804 | 0.564 | 0.005 | 1 |
| | | | | | Sr4 | 12b | 0.523 | 0.706 | 0.937 | 1 |
| | | | (Additional Al atom→) | | Al | 4a | 0.038 | 0.038 | 0.038 | 1 |
| 92 | cI56 | $Cu_3S_3Sb$ | $I\bar{4}3m^b$ | 1.0240 | Sb | 8c | 0.270 | 0.270 | 0.270 | 1 |
| | | | | | Cu1 | 12d | 0.25 | 0.5 | 0 | 1 |
| | | | | | Cu2 | 12e | 0.220 | 0 | 0 | 1 |
| | | | | | S | 24g | 0.117 | 0.117 | 0.360 | 1 |
| 94 | cI58 | $Cu_{12}S_{13}Sb_4$ | $I\bar{4}3m^b$ | 1.0391 | Sb | 8c | 0.268 | 0.268 | 0.268 | 1 |
| | | | | | Cu1 | 12d | 0.25 | 0.5 | 0 | 1 |
| | | | | | Cu2 | 12e | 0.215 | 0 | 0 | 1 |
| | | | | | S | 24g | 0.115 | 0.115 | 0.361 | 1 |
| | | | (Additional S atom→) | | S | 2a | 0 | 0 | 0 | 1 |

$B^{(1)}$, multiplicity and Wyckoff letter.
$N^{(2)}$, occupancy.
[a] Space group number 198.
[b] Space group number 217.

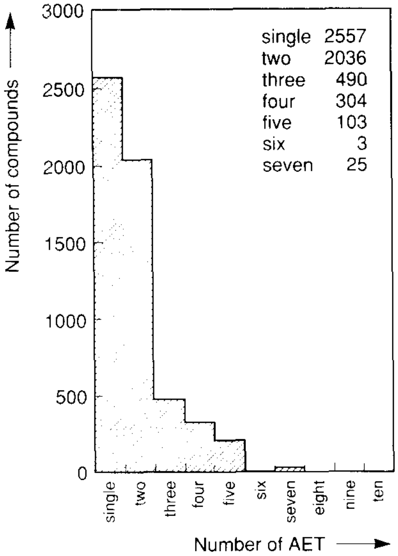


Fig. 9. Number of compounds *vs.* the number of AETs per structure type for the 5521 cubic compounds: single.

TABLE 9

Structure types created by arrangement of the atoms at lower symmetry sites

| No. | Pearson symbol | Structure type | Space group | Multiplicity and Wyckoff letter of the point sets | |
|---|---|---|---|---|---|
| 62 | cF12 | $CaF_2$ | 225 | 4a | 8c |
| | | | | ↓ | ↙ ↘ |
| 20 | cF12 | AlLiSi | 216 | 4a | 4b, 4c |
| 149 | cF16 | NaTl | 227 | 8a | 8b |
| | | | | ↙ ↘ | ↓ |
| 51 | cF16 | $BiF_3$ | 225 | 4a, 4b | 8c |
| | | | | ↓ ↓ | ↙ ↘ |
| 87 | cF16 | $CuHg_2Ti$ | 216 | 4a, 4b | 4c, 4d |
| 89 | cF24 | $Cu_2Mg$ | 227 | 8a | 16d |
| | | | | ↙ ↘ | ↓ |
| 37 | cF24 | $AuBe_5$ | 216 | 4a, 4c | 16e |
| 105 | cP12 | $FeS_2$ | 205 | 4a | 8c |
| | | | | ↓ | ↙ ↘ |
| 151 | cP12 | NiSSb | 198 | 4a | 4a, 4a |
| 63 | cF32 | $Ca_7Ge$ | 225 | 4a, 4b | 24d |
| | | | | ↖ ↗ | ↙ ↘ |
| 65 | cI32 | $Ca_3Hg$ | 217 | 8c | 12d, 12e |

TABLE 10

Structure types created by a translation of coordinates

| Translation | No. | Pearson symbol | Structure type | Space group | Wyckoff positions |
|---|---|---|---|---|---|
| $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | | cF12 | AgAsMg | 216 | 4a, 4c, 4d |
| | 20 | cF12 | AlLiSi | 216 | 4a, 4b, 4c |
| $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | | cP7 | $C_3Nb_4$ | 221 | 1b, 3c, 3d |
| | 166 | cP7 | $S_3U_4$ | 221 | 1a, 3c, 3d |

TABLE 11

Structure types created by a space group reduction (combining two point sets)

| Space group No. 218[a] | | | | | | Space group No. 223[b] | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Atom | $B^{(1)}$ | $x$ | $y$ | $z$ | | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ |
| Na1 | 2a | 0 | 0 | 0 | | K1 | 2a | 0 | 0 | 0 |
| Na2 | 6c | 0.25 | 0.5 | 0 | | K2 | 6d | 0.25 | 0.5 | 0 |
| Al | 6d | 0.25 | 0 | 0.5 | | Si1 | 6c | 0.25 | 0 | 0.5 |
| M1 | 8e | 0.184 | 0.184 | 0.184 | $\}\rightarrow$ | Si2 | 16i | 0.185 | 0.185 | 0.185 |
| M2 | 8e | 0.816 | 0.816 | 0.816 | | | | | | |
| M3 | 24i | 0.000 | 0.306 | 0.116 | | Si3 | 24k | 0 | 0.306 | 0.116 |

M1 = 56at.%Al–44at.%Ge, M2 = 44at.%Al–56at.%Ge and M3 = 17at.%Al–83at.%Ge.

$B^{(1)}$, multiplicity and Wyckoff letter.

[a] cP54, $Al_9Ge_{14}Na_4$, $P\bar{4}3n$.

[b] No. 134, cP54, $K_4Si_{23}$, $Pm\bar{3}n$.

that the AE of Ga3 (mC) is the same as that of Ga1 (hR) with CN = 4, Ga2–Ga4 (mC) have the same AEs as Ga3 (hR) with CN = 6 and the AEs of Ga1–Ga5 (mC) are the same as that of Ga2 (hR) with CN = 7.

A simple example of structure types with the same atomic arrangement is constituted by the structure types of oP8 BFe and oC8 BCr (see Table 14). From the crystallographic description or from the three-dimensional drawing it is not immediately clear that these structure types are identical in their atomic arrangement. Comparing the realized AETs shows that they are geometrically identical (see Figs. 10(a)–10(d) for the next-neighbour histograms and the AET).

As mentioned before, our analysis method finds all Frank–Kasper structures; Shoemaker and Shoemaker [12] have given three cubic structure types with Frank–Kasper coordination polyhedra. These structures are cP8 $Cr_3Si$, cI62 $Al_6Mg_{11}Zn_{11}$ and cF24 $Cu_2Mg$. In addition to these three, we found that cP20 Mn, cP20 $AlAu_4$ and cF24 $AuBe_5$ are also Frank–Kasper structure types, the latter two being derivates of cP20 Mn and cF24 $Cu_2Mg$ respectively. An example of a pseudo-Frank–Kasper structure type is the structure described by Markiv *et al.* [13], namely oP48 $FeGa_2Hf$. The AEs realized in this structure type are Frank–Kasper polyhedra (labelled K, S

TABLE 12

Structure types with equal AETs

| Group | Observed AETs (labels) | No. | Pearson symbol | Structure type |
|---|---|---|---|---|
| 2 environments | A+C | 31 | cI32 | $As_3Co$ |
| | | 105 | cP12 | $FeS_2$ |
| | | 22 | cF56 | $Al_2MgO_4$ |
| | | 143 | cI80 | $Mn_2O_3$ |
| | E+H | 62 | cF12 | $CaF_2$ |
| | | 20 | cF12 | AlLiSi |
| | | 85 | cI96 | $CuFeS_2$ |
| | | 136 | cP96 | $Li_7MnN_4$ |
| | K+Q | 83 | cP8 | $Cr_3Si$ |
| | | 141 | cP20 | Mn |
| | | 11 | cP20 | $AlAu_4$ |
| 3 environments | I+K+O | 100 | cI52 | $Cu_5Zn_8$ |
| | | 17 | cP52 | $Al_4Cu_9$ |
| | | 98 | cF416 | $Cu_{41}Sn_{11}$ |
| 4 environments | K+M+N+Q | 108 | cF408 | $Fe_{11}Zn_{39}$ |
| | | 139 | cF408 | $Mg_{44}Rh_7$ |

TABLE 13

Crystallographic data of two descriptions of $RbGa_7$ with equal AETs

| Space group no. | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ |
|---|---|---|---|---|---|
| 12[a] | Ga1 | 4i | 0.1823 | 0 | 0.4438 |
| | Ga2 | 4i | 0.2169 | 0 | 0.7321 |
| | Ga3 | 4i | 0.4561 | 0 | 0.8679 |
| | Rb | 4i | 0.1949 | 0 | 0.0842 |
| | Ga4 | 8j | 0.1193 | 0.3019 | 0.5561 |
| | Ga5 | 8j | 0.9927 | 0.7905 | 0.2684 |
| 166[b] | Ga1 | 6c | 1/3 | 2/3 | 0.1226 |
| | Ga2 | 18h | 0.7989 | 0.2011 | 0.0187 |
| | Ga3 | 18h | 0.1396 | 0.8604 | 0.0772 |
| | Rb | 6c | 2/3 | 1/3 | 0.1386 |

$B^{(1)}$, multiplicity and Wyckoff letter.

[a] mC32, $RbGa_7$, $C2/m$, $a=1.1432$ nm, $b=0.6603$ nm, $c=1.0259$ nm, $\beta=111.85°$.

[b] hR16, $RbGa_7$, $R\bar{3}m$, $a=0.6600$ nm, $c=2.8563$ nm.

and T), except for the environment of one of the Hf atoms. The code of this AE (CN=17) (see Fig. 11) is $12^{5.0}5^{6.0}$ and it consists, like the code for the Frank–Kasper polyhedra, of 12 vertices adjoining five triangular faces and five vertices adjoining six triangular faces. In our analysis of all symmetries we also observed pseudo-Frank–Kasper polyhedra with the codes $12^{5.0}6^{6.0}$, $12^{5.0}8^{6.0}$ and $12^{5.0}10^{6.0}$.

TABLE 14

Crystallographic data of structure types with identical AETs but with different descriptions

| Space group no. | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ |
|---|---|---|---|---|---|
| 62[a] | B | 4c | 0.036 | 0.25 | 0.610 |
| | Fe | 4c | 0.180 | 0.25 | 0.125 |
| 63[b] | B | 4c | 0 | 0.440 | 0.25 |
| | Cr | 4c | 0 | 0.146 | 0.25 |

$B^{(1)}$, multiplicity and Wyckoff letter.

[a] oP8, BFe, *Pnma*, $a = 0.5495$ nm, $b = 0.2946$ nm, $c = 0.4053$ nm.

[b] oC8, BCr, *Cmcm*, $a = 0.2969$ nm, $b = 0.7858$ nm, $c = 0.2932$ nm.

The complete AE analysis results of all structure types given in ref. 14, which is complete with data up to the end of 1989, is published by the American Society for Materials [15]. In this *Atlas of Crystal Structure Types for Intermetallic Phases* we give for each structure type the crystal data, the complete cell contents and a description of the atomic environments, complete with a three-dimensional drawing of structure, two projections and drawings of all AEs.

## 6. Structure types with "improbable" interatomic distances

A structure determination is likely to be correct only when the interatomic distances are neither too short nor too long. Blind application of HISPOLY or equivalent computer programs for calculating interatomic distances from published crystal structure data, however, can simulate distances which are too short in a structure type containing partly occupied point sets. And although many of these structures have been published incorrectly, *e.g.* due to printing errors, we observed some cases in which these inconsistencies can be removed.

If the seemingly too short distances occur between atoms of the same partly occupied point set, the inconsistency can be removed when the occupancies are 0.5 or less. Physically, this means that the partly occupied point set(s) cannot be occupied truly statistically. In fact, the short-range atomic arrangement corresponds to a lower symmetry and it is this short-range arrangement that varies statistically between the possible enantiomorphs. The energy difference between one enantiomorph and the average structure is obviously so small that the highest entropy modification will be frozen in at low temperatures.

If certain atoms are distributed over two point sets with fractional occupancies, say 0.86 and 0.14, then no simple ordered enantiomorph can be found. The only ordering principle is an exclusion principle preventing simultaneous occupation of sites which are too close, *e.g.* cF72 $FeS_4Yb_2$ and cF312 $Ag_8GeTe_6$.

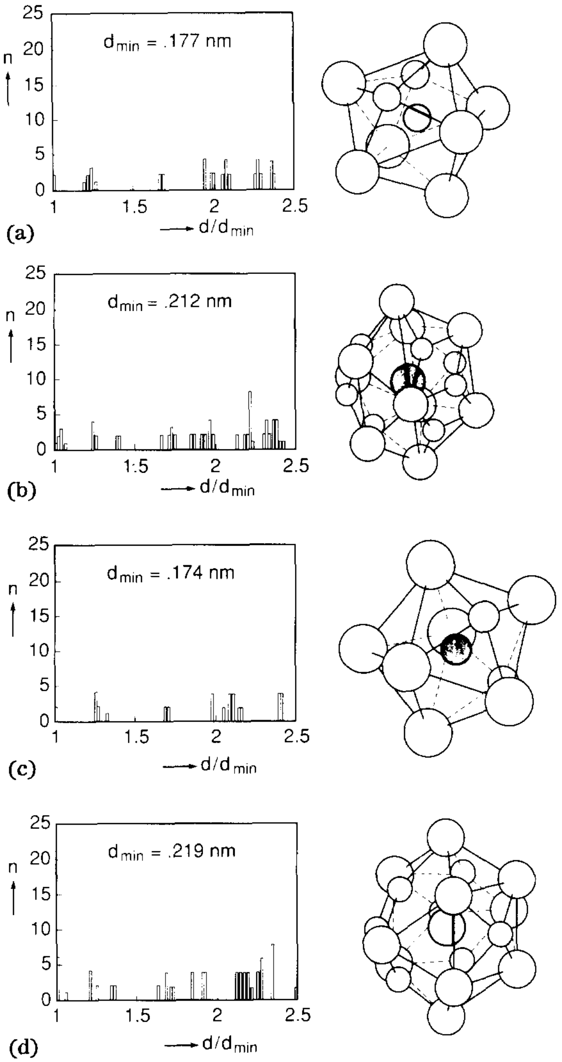


Fig. 10. The AET as observed (a), (b) in oP8 BFe and (c), (d) in oC8 BCr (the B atoms are drawn smaller than the Fe atoms for a better visualization of the AET).

In hydrogen (deuterium)-containing structures we observed improbable interatomic distances, either too long (D–D) or too short (D–M). Because of 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 following three parent structures: 144 cF116 $Mn_{23}Th_6$, 89 cF24 $Cu_2Mg$ and 172 cI2 W.

It is beyond the scope of this work to find the possible ordered structure types. In Table 15 we have listed 21 structure types in which such ordering could in principle occur and 12 hydrides. We would like to stress that, in

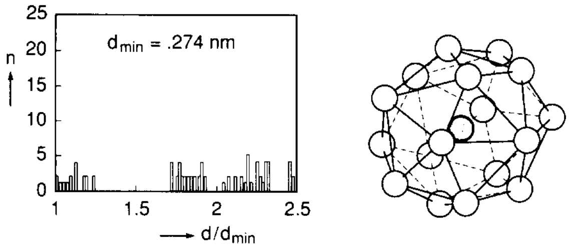


Fig. 11. A typical example of a pseudo-Frank–Kasper polyhedron with the code $12^{5.0}5^{6.0}$.

TABLE 15

Structure types with seemingly improbable interatomic distances

| No. | Pearson symbol | Structure type | No. of representatives | Calculated shortest interatomic distance (nm)[a] |
|---|---|---|---|---|
| 99 | cF28 | $Cu_3Te_2$ | 1 | 0.068 (1) |
| 58 | cF36 | $C_2La$ | 1 | 0.073 (1) |
| 74 | cF44 | $CeH_3$ | 2 | 0.033 (3) |
| 96 | cF44 | $Cu_9Se_5$ | 2 | 0.136 (1) |
| 50 | cF72 | $BiCu_9S_6$ | 3 | 0.093 (1) |
| 106 | cF72 | $FeS_4Yb_2$ | 3 | 0.231 (2) |
| 90 | cF76 | $Cu_4P_{10}Sn$ | 1 | 0.080 (2) |
| 81 | cF120 | $Cr_4H_7Zr_2$ | 1 | 0.177 (3) |
| 101 | cF144 | $Dy_5Pd_2$ | 5 | 0.110 (1) |
| 122 | cF152 | $H_8Mn_{23}Y_6$ | 2 | 0.173 (3) |
| 128 | cF160 | $H_9V_4Zr_2$ | 3 | 0.171 (3) |
| 91 | cF196 | $Cu_7S_4$ | 1 | 0.006 (1) |
| 119 | cF196 | $H_{16}Mn_{23}Th_6$ | 1 | 0.175 (3) |
| 120 | cF200 | $H_{16}Mn_{23}Th_6$ | 1 | 0.228 (3) |
| 5 | cF220 | $Ag_9GaSe_6$ | 1 | 0.049 (1) |
| 103 | cF244 | $Fe_{23}H_8Ho_6$ | 1 | 0.076 (3) |
| 123 | cF248 | $H_{18}Mn_{23}Y_6$ | 1 | 0.158 (3) |
| 86 | cF256 | $Cu_5FeS_4$ | 1 | 0.035 (1) |
| 121 | cF292 | $H_{30}Mn_{23}Th_6$ | 1 | 0.306 (3) |
| 6 | cF312 | $Ag_8GeTe_6$ | 1 | 0.044 (2) |
| 124 | cF344 | $H_{23}Mn_{23}Y_6$ | 1 | 0.225 (3) |
| 102 | cF436 | $Fe_{23}H_{16}Ho_6$ | 1 | 0.044 (3) |
| 43 | cF1936 | $B_{66}Y$ | 1 | 0.107 (2) |
| 127 | cI14 | $HV_2$ | 1 | 0.111 (3) |
| 9 | cI20 | $Ag_2S$ | 1 | 0.122 (2) |
| 34 | cI54 | $As_7Hg_4S_{12}$ | 1 | 0.126 (2) |
| 162 | cI182 | $Rh_{14}Sc_{57}$ | 1 | 0.102 (2) |
| 72 | cI184 | $Cd_6Y$ | 1 | 0.173 (1) |
| 80 | cP26 | Cr | 1 | 0.005 (1) |
| 69 | cP54 | $Cd_5Pt$ | 1 | 0.076 (2) |
| 146 | cP64 | $N_2$ | 1 | 0.038 (1) |
| 14 | cP72 | $Al_6CaTe_{10}$ | 1 | 0.149 (2) |
| 39 | cP76 | $Au_9In_4$ | 1 | 0.036 (1) |

[a](1), enantiomorphic principle; (2), exclusion principle; (3), filled-up structure.

TABLE 16

Structure types with highly improbable interatomic distances

| No. | Pearson symbol | Structure type | No. of representatives | Example of an improbable interatomic gap | Distance (nm) |
|---|---|---|---|---|---|
| 64 | cF48 | $Ca_{33}Ge$ | 2 | Ca–M | 0.255 |
| 148 | cF160 | $NaSi_{14}$ | 1 | Na–Si | 0.225 |
| | | | | Na–Si | 0.390 |
| 132 | cF180 | $In_2Te_3$ | 1 | Te–Te | 0.437 |
| 7 | cF336 | $Ag_8GeTe_6$ | 1 | Ag–Te | 0.186 |
| 21 | cF1832 | $Al_3Mg_2$ | 1 | Al–Mg | 0.750 |
| 43 | cF1880 | $B_{66}Th$ | 1 | B–B | 0.147 |
| 35 | cI46 | $As_8Hg_9S_{24}$ | 1 | Tl–S | 0.386 |
| 110 | cI168 | $Ga_4HfNi_2$ | 1 | M–M | 0.163 |
| 18 | cI276 | $Al_{19}Fe_4MnSi_2$ | 1 | M–M | 0.063 |
| 70 | cI392 | $Cd_5Pt$ | 1 | Cd–Cd | 0.241 |
| 154 | cP64 | $Pb_4S_9Sb_2Sn$ | 1 | M–S | 0.304 |

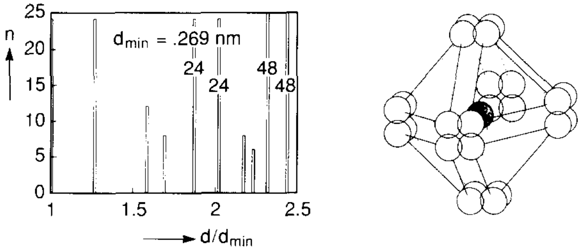


Fig. 12. A typical example of an AE observed in a structure type with seemingly improbable short distances.

those cases where nature realizes such ordering, the structure type represents an average situation of at least two different "pure" single phases. Those structure types represent a rather "exotic" group of structures which have in general only one representative.

For the structure types given in Table 16, those with highly improbable interatomic distances, the same holds that they have only one representative.

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 four 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. This simplification led in all cases to known structure types with many representatives. Examples of redescribed structure types are given in Table 17.

TABLE 17

Crystallographic data of redescribed structure types with originally partly occupied point sets

| Case | Old description | | | | | | | New description | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ | $N^{(2)}$ | | Atom | $B^{(1)}$ | $x$ | $y$ | $z$ | $N^{(2)}$ |
| A | Cr1 | 1a | 0 | 0 | 0 | 1 | } → | Cr1 | 2a | 0 | 0 | 0 | 1 |
| | Cr2 | 1b | 0.5 | 0.5 | 0.5 | 1 | } | | | | | | |
| | Cr3 | 24l | 0.248 | 0.040 | 0.510 | 0.25 | → | Cr2 | 6c | 0.25 | 0 | 0.5 | 1 |
| B | Ce | 4a | 0 | 0 | 0 | 1 | | Ce | 4a | 0 | 0 | 0 | 1 |
| | D1 | 8c | 0.25 | 0.25 | 0.25 | 1 | | D1 | 8c | 0.25 | 0.25 | 0.25 | 1 |
| | D2 | 32f | 0.470 | 0.470 | 0.470 | 0.10 | → | D2 | 4b | 0.5 | 0.5 | 0.5 | 0.80 |
| C | Au1 | 4e | 0.608 | 0.608 | 0.608 | 1 | | Au1 | 4e | 0.608 | 0.608 | 0.608 | 1 |
| | Au2 | 4e | 0.834 | 0.834 | 0.834 | 1 | | Au2 | 4e | 0.834 | 0.834 | 0.834 | 1 |
| | Au3 | 4e | 0.324 | 0.324 | 0.324 | 1 | | Au3 | 4e | 0.324 | 0.324 | 0.324 | 1 |
| | In | 4e | 0.121 | 0.121 | 0.121 | 1 | | In | 4e | 0.121 | 0.121 | 0.121 | 1 |
| | Au4 | 6f | 0.358 | 0 | 0 | 1 | | Au4 | 6f | 0.358 | 0 | 0 | 1 |
| | Au5 | 6g | 0.857 | 0.5 | 0.5 | 1 | | Au5 | 6g | 0.856 | 0.5 | 0.5 | 1 |
| | M1 | 24j | 0.826 | 0.800 | 0.536 | 0.5 | → | M1 | 12i | 0.813 | 0.813 | 0.536 | 1 |
| | M2 | 24j | 0.332 | 0.303 | 0.031 | 0.5 | → | M2 | 12i | 0.318 | 0.318 | 0.031 | 1 |
| D | La | 4b | 0.5 | 0.5 | 0.5 | 1 | | La | 4a | 0 | 0 | 0 | 1 |
| | C | 32f | 0.061 | 0.061 | 0.061 | 0.25 | → | C | 8c | 0.561 | 0.561 | 0.561 | 1 |
| | | | | | Translation → 0.5, 0.5, 0.5 | | | | | | | | |

$B^{(1)}$, multiplicity and Wyckoff letter; $N^{(2)}$, occupancy.

Case A: old description, no. 80, cP26, Cr, space group no. 200, $Pm\bar{3}$; new description, no. 83, cP8, $Cr_3Si$ type, space group no. 223, $Pm\bar{3}m$.

Case B: old description, no. 74, cF44, $CeH_3$, space group no. 225, $Fm\bar{3}m$; new description, cF16, $BiF_3$ type, space group no. 225, $Fm\bar{3}m$.

Case C: old description, no. 39, cP76, $Au_9In_4$, space group no. 215, $P\bar{4}3m$, $M1$ = 12.5at.%Au–37.5at.%In, $M2$ = 37.5at.%Au–12.5at.%In; new description, no. 17, cP52, $Al_4Cu_9$ type, space group no. 215, $P\bar{4}3m$, $M1$ = 25at.%Au–75at.%In, $M2$ = 75at.%Au–25at.%In.

Case D: old description, no. 58, cF36, $C_2La$, space group no. 225, $Fm\bar{3}m$; new description, no. 105, cP12, $FeS_2$ type, space group no. 205, $Pa\bar{3}$.

In Fig. 12 we demonstrate the effect of a wrong description, due to a partly occupied point set, by showing the environment of the 4b position of cF36 $C_2La$. The AE is in principle an octahedron, in which each corner position is split into four positions, each occupied by 25%. A similar effect can be described with our proposed new description and using an anisotropic temperature factor.

## 7. Conclusions

Our analysis shows that in 12 790 (92%) out of 13 917 investigated AEs, in cubic systems, nature prefers one of the 21 most symmetrical AETs shown in Fig. 5. Remarkably, these 21 AETs are equally often found in single-environment up to polyenvironment groups, meaning that even in complex structures symmetrical AETs are preferred. Nature obviously prefers the formation of the geometrically simplest structures, preferably containing one or two 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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