

5. $(6^3)_6(8^3)_2(6^38^3)_6-b$ Space group $P6_3/m$ (No. 176)
 $Z' = 14$

$$v_3 \begin{cases} 6(h) (xy\frac{1}{4}) & x=0.03 \ y=0.33 \\ 2(d) (\frac{2}{3}\frac{1}{4}) \end{cases}$$

$$v_4 \ 6(h) (xy\frac{1}{4}) \ x=0.77 \ y=0.17$$

$$c : a = 0.382^*$$

6. $(8^3)_8(8^6)_6$ Space group $Pm3n$ (No. 223) $Z' = 14$

$$v_3 \ 8(e) (\frac{1}{4}\frac{1}{4}\frac{1}{4})$$

$$v_4 \ 6(c) (\frac{1}{4}0\frac{1}{2})$$

Examples do not appear to be known of structures based on the nets 2 and 4; examples of the other nets include the following:

Net 1. No example is known of an A_3X_4 structure based on the most symmetrical (cubic) configuration of this net, but the structure of In_2CdSe_4 is a superstructure in which the non-equivalence of the tetrahedrally coordinated In and Cd atoms results in lowering of the symmetry to $P\bar{4}2m$, in which the positions occupied are:

$$v_3 \ 4(n) (xxz) \ x=z=\frac{1}{4}$$

$$v_4 \begin{cases} 2(e) (\frac{1}{2}00, 0\frac{1}{2}0) \\ 1(c) (00\frac{1}{2}). \end{cases}$$

Net 3. The most symmetrical form of this net represents the structure of $\beta-Cu_2HgI_4$ and related compounds. In $\beta-Ag_2HgI_4$, the same positions are occupied by the Hg and I atoms as in the copper compound, but the distribution of the Ag atoms in two sets of equivalent positions leads to lower symmetry, $I\bar{4}$ instead of $I\bar{4}2m$:

* Values of variable parameters are those for $\beta = Si_3N_4$.

$\beta-Cu_2HgI_4$	$\beta-Ag_2HgI_4$
Space group $I\bar{4}2m$ (No. 121)	Space group $I\bar{4}$ (No. 82)
Hg in 2(a) (000)	Hg in 2(a) (000)
Cu in 4(d) $(0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2})$	Ag in 2(b) $(00\frac{1}{2})$
I in 8(i) $(\frac{1}{4}\frac{1}{4}\frac{3}{8})$	and 2(c) $(0\frac{1}{2}\frac{1}{2})$
	I in 8(g) $(\frac{1}{4}\frac{3}{8}\frac{3}{8})$.

Net 5. The most symmetrical configuration of this net forms the basis of the structure of $\beta-Si_3N_4$ (Goodman & O'Keeffe, 1980). In $\alpha-Si_3N_4$ there is a less-regular arrangement of the SiN_4 groups along the c axis requiring a doubled c parameter, $4Si_3N_4$ in the unit cell, and space group $P31c$ (Marchand, Laurent & Lang, 1969). The structures of the two polymorphs of Ge_3N_4 also are based on this net.

Numerous compounds A_2BX_4 have structures based on this net distorted in various ways from the most symmetrical configuration described above. They include ternary oxides (for example, Li_2CrO_4 , Zn_2SiO_4 , Zn_2GeO_4) and ternary fluorides (Li_2BeF_4 , Li_2ZnF_4). In compounds A_2BX_4 the non-equivalence of the two kinds of tetrahedrally coordinated atoms leads to more-complex and less-symmetrical variants of the structure. For example, the mineral phenacite, with ideal composition Be_2SiO_4 , is rhombohedral (space group $R\bar{3}$) with 18 formula weights in the unit cell (that is, $Z' = 126$).

Net 6. This net represents the arrangement of Pt and O atoms in the structure assigned to $(Pt_3O_4)Na_x$.

References

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On integrating the techniques of direct methods with anomalous dispersion. I. The theoretical basis.

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Abstract

In equation (2.7) of Hauptman [*Acta Cryst.* (1982), A38, 632-641] $2\theta_{jH}$ should be replaced by $2\delta_{jH}$. On the seventh line of equation (3.34), $C_H C_K C_L - C_H S_K S_L$ should be

replaced by $C_H C_K C_L + C_H S_K S_L$. On the sixth line of equation (3.51), replace $R_1 R_2 R_3 \cos \zeta_2$ by $R_1 R_2 R_3 \cos \zeta_2$. On the line immediately following equation (3.54), $\omega_j B_j$ should be replaced by $\omega_j B_j$.