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# SHORT COMMUNICATIONS

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about* 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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## Note on 3D (3, 4)-connected nets.

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**Abstract**

Three new 3D (3, 4)-connected nets are described belonging to the special family of nets in which each 3-connected point is connected to three 4-connected points and each 4-connected point is connected to four 3-connected points.

In earlier accounts of three-dimensional nets (Wells, 1977, 1979) it was noted that a special family of 3D (3, 4)-connected nets comprises those in which every 3-connected point is connected to three 4-connected points and every 4-connected point to four 3-connected points. These nets represent actual or possible structures of compounds $A_3X_4$ in which $A$ and $X$ are the 4- and 3-connected atoms respectively. Since the unit cell in an ordered structure must contain one or more $A_3X_4$ the total number $Z'$ of 3- and 4-connected atoms must be a multiple of 7, that is, $Z'=7Z$ for a unit cell containing $Z(A_3X_4)$. The only nets of the $Z'=7m$ family that were described previously were one cubic net with $Z'=7$ and two nets with $Z'=14$. A by-product of a survey of tetrahedral structures (Wells, in preparation) was the recognition of three more nets of the $Z'=7m$ family, all with $Z'=14$. These are the nets 2, 3 and 4 listed below. The structures based on net 3 have been known for some time, but were not described as examples of a net of this type.

Accordingly we may now list six nets of the $Z'=7m$ family. The first five can be built with regular tetrahedral coordination of the 4-connected $A$ atoms and are illustrated as structures built from regular tetrahedra in the survey referred to above. In the most symmetrical configuration of the sixth net there is square coplanar coordination of the 4-connected points. The coordination of the 3-connected points is exactly or approximately trigonal coplanar in nets 6 and 5 respectively but pyramidal in nets 1-4. The two cubic nets 1 and 6 are the only two of this family in which all 3-connected points are symmetrically equivalent and all 4-connected points are symmetrically equivalent. The detailed descriptions of the most symmetrical configurations of the nets are as follows:

1. $(6^3)_4(6^28^4)_3$ Space group $P\bar{4}3m$ (No. 215) $Z'=7$

$$v_3\ 4(e)\ (xxx)\ x=\tfrac{1}{4}$$
$$v_4\ 3(d)\ (\tfrac{1}{2}00)$$

2. $(6^3)_6(8^3)_2(6^38^3)_6-a$ Space group $P6_3mc$ (No. 186) $Z'=14$

$$v_3\begin{cases}2(b)\ (\tfrac{1}{3}\tfrac{2}{3}z)\ z=\tfrac{1}{2}\\ 6(c)\ (x\bar{x}z)\ x=\tfrac{1}{6}\ z=0\end{cases}$$
$$v_4\ 6(c)\ (x\bar{x}z)\ x=\tfrac{1}{6}\ z=\tfrac{3}{8}$$
$$c:a=\sqrt{2}/\sqrt{3}$$

3. $(6^3)_8(6^38^3)_2(6^28^4)_4$ Space group $I\bar{4}2m$ (No. 121) $Z'=14$

$$v_3\ 8(i)\ (xxz)\ x=\tfrac{1}{4}\ z=\tfrac{3}{8}$$
$$v_4\begin{cases}2(a)\ (000)\\ 4(d)\ (0\tfrac{1}{2}\tfrac{1}{4})\end{cases}$$
$$c:a=2$$

4. $(6^3)_2(6.8^2)_2(6^3)_4(6^38^3)_2(6^48^2)_4$ Space group $Pmn2_1$ (No. 31) $Z'=14$

$$v_3\begin{cases}2(a)\ (0yz)\ y=\tfrac{1}{3}\ z=\tfrac{15}{16}\\ 2(a)\ (0yz)\ y=\tfrac{2}{3}\ z=\tfrac{7}{16}\\ 4(b)\ (xyz)\ x=\tfrac{1}{4}\ y=\tfrac{1}{6}\ z=\tfrac{7}{16}\end{cases}$$
$$v_4\begin{cases}2(a)\ (0yz)\ y=\tfrac{1}{3}\ z=\tfrac{9}{16}\\ 4(b)\ (xyz)\ x=\tfrac{1}{4}\ y=\tfrac{1}{6}\ z=\tfrac{1}{16}\end{cases}$$
$$a:b:c=2/\sqrt{3}:1:2\sqrt{2}/3$$

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

$$v_3\begin{cases}6(h)\ (xy\tfrac{1}{4})\ \ x=0{\cdot}03\ \ y=0{\cdot}33\\ 2(d)\ (\tfrac{2}{3}\tfrac{1}{3}\tfrac{1}{4})\end{cases}$$

$$v_4\ \ 6(h)\ (xy\tfrac{1}{4})\ \ x=0{\cdot}77\ \ y=0{\cdot}17$$

$$c:a=0{\cdot}382^*$$

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

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

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

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:

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

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

*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 $I\bar{4}2m$:

| $\beta$-$Cu_2HgI_4$ | $\beta$-$Ag_2HgI_4$ |
|---|---|
| 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 $4(d)$ $(0\tfrac{1}{2}\tfrac{1}{4},\tfrac{1}{2}0\tfrac{1}{4})$ | Ag in $2(b)$ $(00\tfrac{1}{2})$ |
| I in $8(i)$ $(\tfrac{1}{4}\tfrac{1}{4}\tfrac{3}{8})$ | and $2(c)$ $(0\tfrac{1}{2}\tfrac{1}{4})$ |
| | I in $8(g)$ $(\tfrac{1}{4}\tfrac{1}{4}\tfrac{3}{8})$. |

*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 $(Pt_3O_4)Na_x$.

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

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

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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), $C_HC_KC_L-C_HS_KS_L$ should be replaced by $C_HC_KC_L+C_HS_KS_L$. On the sixth line of equation (3.51), replace $R_{\bar{1}}R_{\bar{2}}R_{\bar{3}}\cos\zeta_2$ by $R_{\bar{1}}R_2R_{\bar{3}}\cos\zeta_2$. On the line immediately following equation (3.54), $\omega_jB_{\bar{j}}$ should be replaced by $\omega_j, B_{\bar{j}}$.