

A structure based on a 3-connected net may be formed from any units which can be connected to three others, for example, tetrahedral AX_4 groups sharing three vertices or an edge and two vertices, or from octahedral AX_6 groups sharing three vertices, three edges, or other combination (totalling three) of vertices, edges, and faces. It might therefore be expected that such structures, particularly those built from octahedra, would provide many examples of 3-connected nets. A preliminary (unpublished) survey of octahedral AX_n and A_2X_n structures has revealed a considerable number of structures based on uniform and Archimedean 3-connected nets, including:

$8^3\text{-a}:A_2X_7$	6.10 ²	A_2X_9, AX_4, A_2X_7
$10^3\text{-a}:A_2X_7, AX_3$	4.14 ^{2-a}	A_2X_9
$10^3\text{-b}:A_2X_9, AX_4, A_2X_7, AX_3$	4.14 ^{2-b}	AX_4
$10^3\text{-c}:A_2X_9, AX_3, A_2X_7$	4.8.10-a	AX_4

However, no examples of any of these structures appear to be known; indeed, very few examples of

structures of any kind based on Archimedean 3-connected nets are known (Wells, 1979, p. 15). It was the study of these octahedral structures that led to the derivation of the net 4.14^{2-b}, and this in turn suggested the nets of Figs. 2, 3, 4, and 6, in all of which the 4-gon circuits are perpendicular to the plane of projection and are shown as double lines. The net of Fig. 6 is of special interest as the only example at present known of a net 4.16²; it continues the series which starts with the cube (4.4²), truncated octahedron (4.6²), plane net (4.8²), double layer (4.10²), and the 3D nets 4.12² and 4.14².

References

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SHORT COMMUNICATION

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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A note on the structure of $TiMnSi_2$ and the tetrahedrally close-packed 'pentagon–sigma' structure. By CLARA BRINK SHOEMAKER, *Department of Chemistry, Oregon State University, Corvallis, OR 97331, USA*

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Abstract

The hypothetical tetrahedrally close-packed (t.c.p.) structure, which is a pentagon–triangle analogue of the hexagon–triangle σ phase, mentioned by Steinmetz, Venturini, Roques, Engel, Chabot & Parthé in their paper on the structure of $TiMnSi_2$ [*Acta Cryst.* (1982), **B38**, 2103–2108], has actually been found to exist in the W–Fe–Si system at approximate composition W_2FeSi by Kripyakevich & Yarmolyuk [*Dopov. Akad. Nauk. Ukr. RSR Ser. A* (1974), **36**, 460–463]. This 'pentagon–sigma' structure is one of four t.c.p. structures of composition R_6X_7 [R represents atoms with coordination number (CN) > 12, and X atoms with CN = 12]. The other structures are the M phase, the μ phase, and a hypothetical structure which has a projection almost identical to the projection of the hypothetical structure given in Fig. 3(b) of Steinmetz *et al.* (1982).

Steinmetz *et al.* (1982) observe that the c projection of $TiMnSi_2$ and $TiFeSi_2$ resembles closely the projection of a pentagon–triangle analogue, given in Fig. 6(b) in Shoemaker & Shoemaker (1969), of the hexagon–triangle σ phase. This 'pentagon–sigma' structure has actually been found to occur in the W–Fe–Si system [composition $W_6(Fe_{0.465}Si_{0.465}W_{0.07})_7$] by Kripyakevich & Yarmolyuk (1974). The space groups for $TiMnSi_2$ and the 'pentagon–sigma' structures are

the same ($Pbam$, a and b interchanged, c approximately doubled in $TiMnSi_2$).

Although the c projections of the $TiMnSi_2$ and the 'pentagon–sigma' structures are almost identical, Steinmetz *et al.* (1982) point out that the structures are actually quite different: $TiMnSi_2$ has three secondary layers for four main layers, whereas the tetrahedrally close-packed (t.c.p.) structure has an equal number of secondary and main layers. The $TiMnSi_2$ structure contains octahedra of Si atoms (surrounding metal atoms), whereas the 'pentagon–sigma' structure has only possible Si–Si contacts through sites of mixed W, Fe, Si or Fe, Si occupancy. With 25 at.% Si 'W₂FeSi' is at the upper limit of Si content of t.c.p. structures described before.

The 'pentagon–sigma' structure was first proposed as a hypothetical structure by Frank & Kasper (1959) as entry 8 in their Table 3. They also proposed a hypothetical structure (entry 9 in the same table), which is the all-pentagon analogue of the pentagon–hexagon structure of the P phase. That hypothetical structure was later found to occur as the M phase in the Nb–Ni–Al system ($Nb_{48}Ni_{39}Al_{13}$, Shoemaker & Shoemaker, 1967). The 'pentagon–sigma' and the M phase are very similar to the t.c.p. μ phase (W₆Fe₇, Arnfelt & Westgren, 1935). The formula for all three phases may be written as R_6X_7 , where R represents atoms with CN > 12, and X atoms with CN = 12 (Yarmolyuk & Kripyakevich,

1974). The ratios of atoms with CN16, CN15, CN14 and CN12 are 2:2:2:7 for all three structure types.

The hypothetical structure shown by Steinmetz *et al.* (1982) in Fig. 3(b) has the same tessellations for the secondary network ($4^2.3^3$) as does the t.c.p. μ phase, mentioned above, and shown in Shoemaker & Shoemaker (1969) in Fig. 6(a). Its projection, however, is not identical to the μ -phase projection, which would be obtained if the transformation mechanism described by Steinmetz *et al.* to obtain Fig. 3(b) were performed on a structural slab running in the **b** direction, rather than in the **a** direction. {In this case the middle slab also has to be shifted in the [001] direction and infinite rows of atoms similar to those in Fig. 3(b) are not formed.}

The hypothetical t.c.p. structure (with two main layers and two secondary layers), which has a *c* projection almost identical to the hypothetical structure in Fig. 3(b), is also a four-layer structure when projected down [130] of TiMnSi_2 . When viewed in that direction the main layers consist of alternating rows of hexagons and pentagons, and the

secondary layers have 3^6 tessellations. It is the hypothetical t.c.p. structure shown in Fig. 7(b) of Shoemaker & Shoemaker (1969). It is a fourth t.c.p. structure that may be formulated as R_6X_7 , and that has the same ratios of atoms with the different coordination types as mentioned above.

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Chemical Nomenclature

The attention of authors is drawn to the following recommendations of the IUPAC Commission on Nomenclature of Organic Chemistry: *The Designation of Non-Standard Classical Valence Bonding in Organic Nomenclature* [*Pure Appl. Chem.* (1982), **54**, 217–227], *Revision of the Extended Hantzsch–Widman System of Nomenclature for Heteromonocycles* [*Pure Appl. Chem.* (1983), **55**, 409–416]; and to the following recent recommendations of the IUPAC–IUB Joint Commission on Biochemical Nomenclature: *Symbols for Specifying the Conformation of Polysaccharide Chains* [*Eur. J. Biochem.* (1983), **131**, 5–7], *Abbreviations and Symbols for the Description of Conformation of Polynucleotide Chains* [*Eur. J. Biochem.* (1983), **131**, 9–15].

Authors are reminded that, wherever possible, chemical nomenclature in the Union's journals should conform to IUPAC rules. Basic rules for the nomenclature of inorganic chemistry are given in *Nomenclature of Inorganic Chemistry* (1970) ('The Red Book'), London: Butterworths and, for organic chemistry, in the two volumes *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, & H* (1979) ('The Blue Book'), Oxford: Pergamon Press and *Biochemical Nomenclature and Related Documents* (1978), London: Biochemical Society. For further details on nomenclature requirements see *Notes for Authors* [*Acta Cryst.* (1983), **A39**, 174–186].

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Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Extended linear chain compounds, Vol. 3. Edited by J. S. MILLER. Pp. xviii + 561. New York and London: Plenum Press, 1983. Price US \$55.00.

This third volume represents another ten review papers on one-dimensional chain compounds, and I can repeat the comment made already by H. Boller (1983) in his review of the first and second volumes (*Acta Cryst.* **B39**, 287), 'Each contribution covers its subject independently and can therefore be studied at the reader's choice'.

The first chapter describes the experimental results of Gillespie's (1971) prediction, 'It seemed reasonable to suppose that, if two mercury atoms could be bonded together (Hg_2^{2+}), it might be possible to prepare cations containing three or even more mercury atoms covalently bonded together'. Chapter 2 deals extensively and systematically with the metal–metal chain bondings in hexagonal close-packed anion spheres (hexagonal perovskites); ferromagnetic properties of these compounds are dealt with in chapter 3. Chapters 4 and 5 turn to stacked organic charge-transfer complexes in which magnetic resonance results predominate amongst the many physical properties of these stacking