

change of their positional coordinates, have changed their affiliation, thus belonging to another unit.

Conclusion

It follows from this study that the notion of nested polyhedra units is a purely geometrical concept. It should be emphasized that the interatomic distances within a unit are not necessarily shorter than those between units. Further, the nested polyhedra units must not be confused with the coordination polyhedra which are defined around the atoms. This geometric description offers nevertheless great advantages for structures with high symmetry. As each polyhedron is formed by atoms from one equipoint, it is possible to find rapidly the type of polyhedron, as well as its centre, from the atom coordinates. Further, since all the nested polyhedra are simple and have the same centre, the structure can be visualized and memorized more easily than from descriptions based on arrangements of smaller polyhedra sharing vertices, edges and/or faces. The nested polyhedra concept can thus be useful to describe in a condensed way, and to compare, apparently complicated cubic structures containing a large number of atoms in the unit cell.

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The Related Structures of α -Mn, Sodalite, Sb_2Tl , etc.*

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Abstract

The sodalite structure can be regarded as a three-dimensional framework of corner-connected tetrahedra. By tilting the tetrahedra through various angles

equivalent frameworks in the structures of α -Mn, sodalite and Sb_2Tl , are obtained. The complete structures are obtained by filling the large interstices in these frameworks with various atom groups.

* Editorial note: The similarity between this paper and the two preceding papers, by Hellner & Koch [*Acta Cryst.* (1981), **A37**, 1-6] and by Chabot, Cenzual & Parthé [*Acta Cryst.* (1981), **A37**, 6-11], has been recognized and they have been published together to give an indication of the activity in the field with which they are concerned.

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Introduction

In an earlier paper (Nyman, Andersson, Hyde & O'Keeffe, 1978) rather complicated structures, e.g. VAl_{10} , $\text{W}_3\text{Fe}_3\text{C}$ and Ti_2Ni , were described as pairs of simple interpenetrating frameworks. By the same

Table 1. *The x and z parameters of the atoms in the 24-fold positions forming the tetrahedral framework*

Compound	x	z	α (°)	a_c (Å)	a_o (Å)	Reference
Ideal I	0.1464	0	0	3.414d	—	
Ideal II	$\frac{1}{2}$	$\frac{1}{2}$	45	2.828d	—	
Ideal III	0	0.354	90	1.414d	—	
Sb ₂ Tl ₇	0.151	0	0	3.414d	11.618	(a)
γ -(Mg,Al)	0.159	0	0	3.414d	10.437	(b)
α -Mn	0.14294	0.03457	13.6	3.358d	8.911	(c)
Ti ₂ Re ₂₄	0.144	0.042	16.3	3.333d	9.609	(d)
Zr ₂ Re ₂₄	0.144	0.042	16.3	3.333d	9.645	(e)
Er ₂ Re ₂₄	0.144	0.042	16.3	3.333d	11.23	(f)
χ -phase, Fe ₃₆ Cr ₁₃ Mo ₁₀	0.144	0.042	16.3	3.333d	8.920	(g)
Cr _{17.4} Co _{29.0} Si _{11.6}	0.144	0.042	16.3	3.333d	8.705	(h)
Nb _{14.5} Re _{43.5}	0.140	0.040	15.9	3.337d	9.692	(i)
Binnite, As ₄ Cu ₁₂ S _{13-x}	0.119	0.1442	50.3	2.693d	10.232	(j)
Tetrahedrite, Cu ₁₂ Sb ₄ S ₁₃	0.117	0.140	50.1	2.697d	10.24	(k)
Tetrahedrite	0.1152	0.139	50.3	2.693d	10.398	(l)
Sodalite, Na ₄ Al ₃ Si ₃ O ₁₂ Cl	0.1401	0.0615	23.7	3.246d	8.870	(m)
Hydrosodalite, Na _{7.1} (Al ₆ Si _{2.5} H ₂)O ₂₄ Cl _{0.4} (OH) _{0.7}	0.1374	0.065	23.8	3.244d	8.887	(n)
Häuynite, Na ₃ CaAl ₃ Si ₃ O ₁₂ ·SO ₄	0.136	0.025	10.42	3.381d	9.06	(o)
Helvite, (Mn,Fe,Zn) ₄ Be ₃ Si ₃ O ₁₂ S	0.137	0.084	31.51	3.119d	8.25	(p)
Na-ultramarine, Na _{6.86} Si _{6.35} Al _{6.08} O _{26.2} S _{2.54}	0.136	0.025	10.42	3.381d	9.06	(q)
Li-ultramarine, Li _{4.86} Na _{0.86} Si _{6.35} Al _{6.08} O _{26.2} S _{2.54}	0.143*	0.056	21.4	3.277d	8.68	(q)
Ag-ultramarine, Ag _{5.25} Na _{2.3} Si _{6.2} Al _{5.8} O ₂₄ S _{1.95}	0.136	0.042	17.2	3.325d	8.98	(q)

References: (a) Stokhuyzen, Chieh & Pearson (1977); (b) Taketoshi (1971); (c) Oberteuffer & Ibers (1970); (d) Trzebiatowski & Niemiec (1955); (e) Kripjakevič, Tylkina & Savickij (1960); (f) Kripjakevič & Evdokimenko (1962); (g) Kasper (1954); (h) Gladyshevskij, Kripjakevič & Kuz'ma (1962); (i) Steadman & Nuttall (1964); (j) Edenharter, Koto & Nowacki (1971); (k) Avilov, Imamov & Muradian (1971); (l) Wuensch (1964); (m) Löns & Schulz (1967); (n) Bukin & Marakov (1967); (o) Machatschki (1934); (p) Pauling (1930); (q) Podschus, Hofmann & Leschewski (1936).

* In the original paper (Podschus, Hofmann & Leschewski, 1936), the atomic parameters are given as angles. The angle given as x parameter for the O-atom position in Li-ultramarine is 51.5° which corresponds to $x = 0.143$. In *Strukturbericht* (1936), the erroneous $x = 0.115$ is given.

the two 24-fold positions of the structure of Ti₂Re₂₄ are depicted, to show an example of an intermediate rotation angle, $\alpha = 16.3^\circ$. In tetrahedrite, Fig. 4, the framework is collapsed beyond $\alpha = 45^\circ$, which forces some S atoms closer to each other, 3.258 Å, than the average S—S distance of 3.663 Å.

Interpenetrating structures

If the atoms creating the tetrahedral framework are ignored, the remaining atoms can be thought of as a second structure which interpenetrates the tetrahedral framework.

In the fully open γ -(Mg,Al), the framework cavities are occupied by Mg-centred Al₆ octahedra surrounded by a cube of Al atoms to form a slightly distorted f.c.c. unit, Fig. 2. These 15-atom groups surrounding 000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ are discrete, *i.e.* not connected to each other.

The structure of Sb₂Tl₇, Fig. 5 (Morrall & Westgren, 1934; Stokhuyzen, Chieh & Pearson, 1977), is very close to that of γ -(Mg,Al). The main difference is a change in the x parameter of position 12(e) from $x = 0.233$ in γ -(Mg,Al) to $x = 0.3138$ in Sb₂Tl₇. This change turns the structure of the interstitial groups from approximately f.c.c. to b.c.c.

In Re₂₄Ti₅, the tetrahedral framework though collapsed still accommodates discrete groups of 17 atoms, this time in the shape of a truncated tetrahedron of twelve Re atoms, centred by a Ti atom and capped on

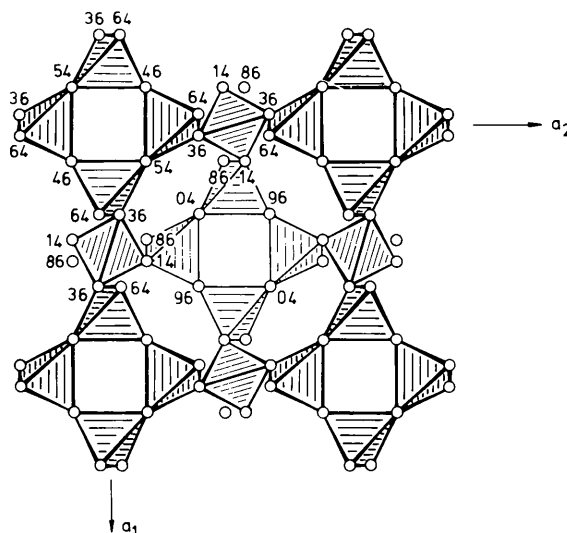


Fig. 3. One of the two 24-fold sets of Re positions in the Re₂₄Ti₅ structure, creating a slightly collapsed tetrahedral framework (*cf.* Fig. 6).

each of its four hexagonal faces by an additional Ti atom. This interpenetrating structure is shown in Fig. 6. The structures of α -Mn and the so-called χ -phase $Fe_{36}Cr_{12}Mo_{10}$ are very similar to the $Re_{24}Ti_5$ structure. In α -Mn all 58 atom positions in the unit cell are occupied by Mn atoms, *i.e.* there are four crystallographically different Mn atoms in α -Mn.

Another way to look at the $Re_{24}Ti_5$ structure is to take the framework tetrahedra as the central tetrahedra of *stellae quadrangulae*, which are completed by the Re atoms in the second 24-fold position. These polyhedra share edges as shown in Fig. 7. To avoid too

close an approach between the closest atoms, *e.g.* the two labelled 22 in the central part of Fig. 7, the *stellae quadrangulae* have to be distorted in a way which can be most clearly seen in the right part of Fig. 7. Even so, this distance remains the shortest Re-Re distance in the structure, 2.419 compared to 2.878 Å for the edge of a *stella quadrangula* (*cf.* 2.761 Å in Re metal).

This array of edge-sharing *stellae quadrangulae* creates truncated tetrahedra which are occupied by Ti atoms and bisdisphenoids which are empty.

The common description of the sodalite structure is that of the tetrahedral framework (described above) which is collapsed around big Cl-centred Na tetrahedra, arranged as in Fig. 8 (Pauling, 1930). However, these tetrahedra can also be thought of as the central tetrahedra of *stellae quadrangulae*, and the interpenetrating structure is then an array of corner-

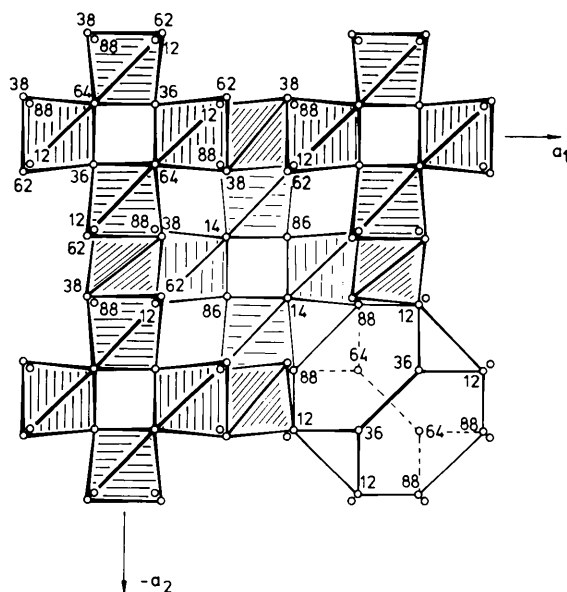


Fig. 4. The 'over-collapsed' tetrahedral framework of tetrahedrite. One of the cavities in the framework is outlined at lower right.

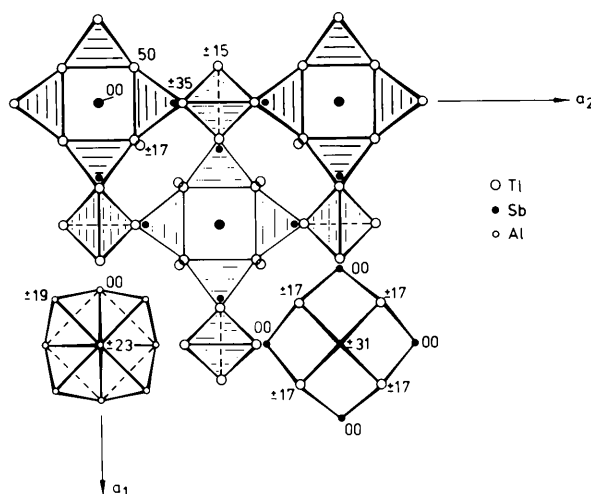


Fig. 5. The structure of Sb_2Ti_7 : the lower right part shows the interpenetrating b.c.c. structure, to be compared with the f.c.c. structure in γ -(Mg,Al) which is inserted at lower left.

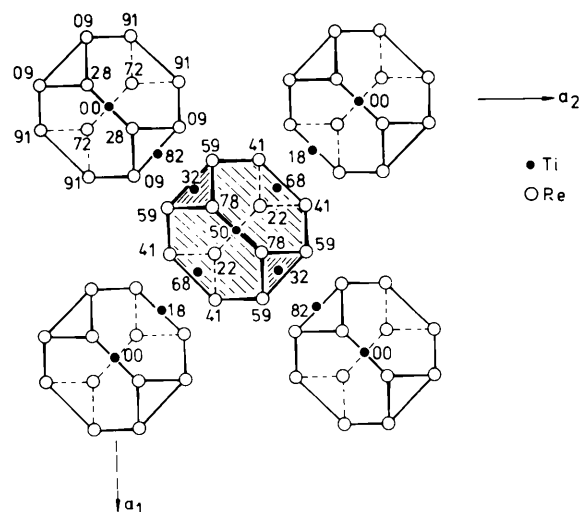


Fig. 6. The remaining part (*cf.* Fig. 3) of $Re_{24}Ti_5$: four-capped truncated tetrahedra.

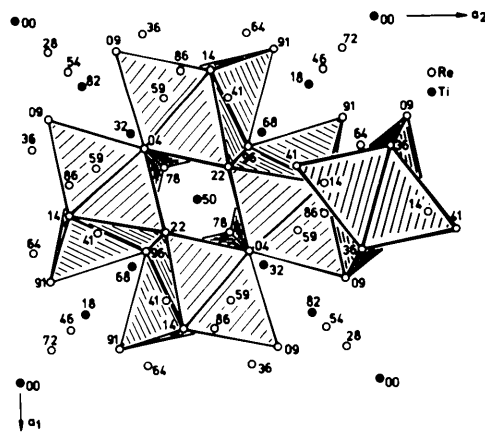


Fig. 7. Some of the edge-sharing *stellae quadrangulae* in $Re_{24}Ti_5$. The necessary twist distortion of this polyhedron can be seen on the right-hand side of the figure.

connected *stellae quadrangulae*, Fig. 9. This second (interpenetrating) structure is the anti-structure of SiF_4 (Nyman & Andersson, 1979), with even more regular *stellae quadrangulae* than in SiF_4 itself. (In a framework of ideal *stellae quadrangulae* the parameter $x = \frac{1}{16} \approx 0.187$, in SiF_4 $x = 0.165$ and in sodalite the corresponding parameter is $x = 0.177$.)

In the closely related h a ynite the Cl atoms are replaced by SO_4 groups, which opens up the tetrahedral framework. Together with their surrounding tetrahedra of (Na,Ca) atoms they can be considered as discrete *stellae quadrangulae*, Fig. 8, or, by analogy with sodalite, a framework of bigger corner-connected *stellae quadrangulae* can be constructed as in Fig. 9. In

this case they are more heavily distorted with the parameter $x = 0.222$. In fact, the distortion makes the polyhedron somewhat closer to a cube, $x = 0.25$, than to a *stella quadrangula*, $x = 0.187$. The interpenetrating structure is approaching an array of corner-connected cubes like the structure of $\beta\text{-Hg}_4\text{Pt}$ (Bauer, Nowotny & Stempfl, 1953).

In tetrahedrite, which is greatly collapsed, the interstitial part of the structure consists of discrete SCu_6 octahedra capped on four faces by Sb atoms, Fig. 10. As mentioned before, the holes of the tetrahedral framework, when fully collapsed, are in the shape of truncated tetrahedra. The SCu_6 octahedra are oriented in such a way that each of the four Sb caps points

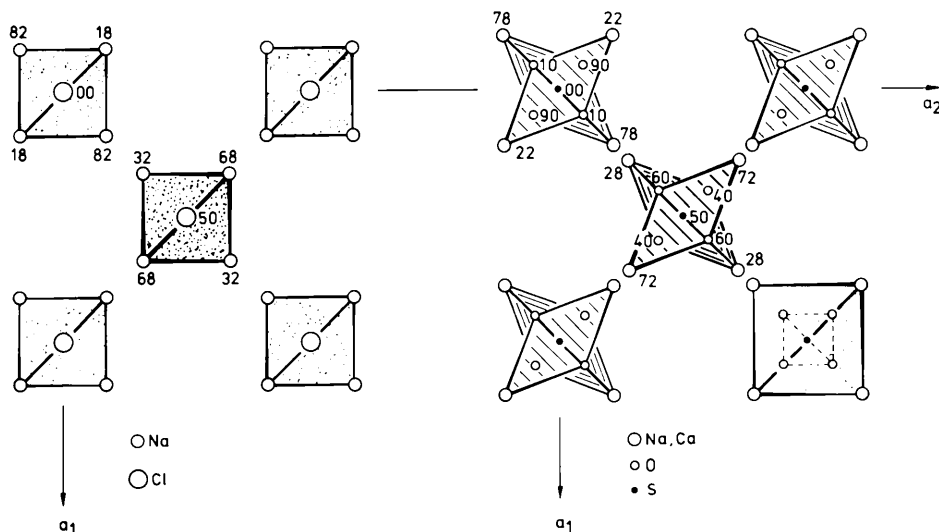


Fig. 8. Left: the interpenetrating structure of sodalite: big ClNa_4 tetrahedra. Right: in h a ynite the Cl atoms of sodalite are replaced by SO_4 tetrahedra, the lower right part shows one Na tetrahedron, comparable with the ones in sodalite.

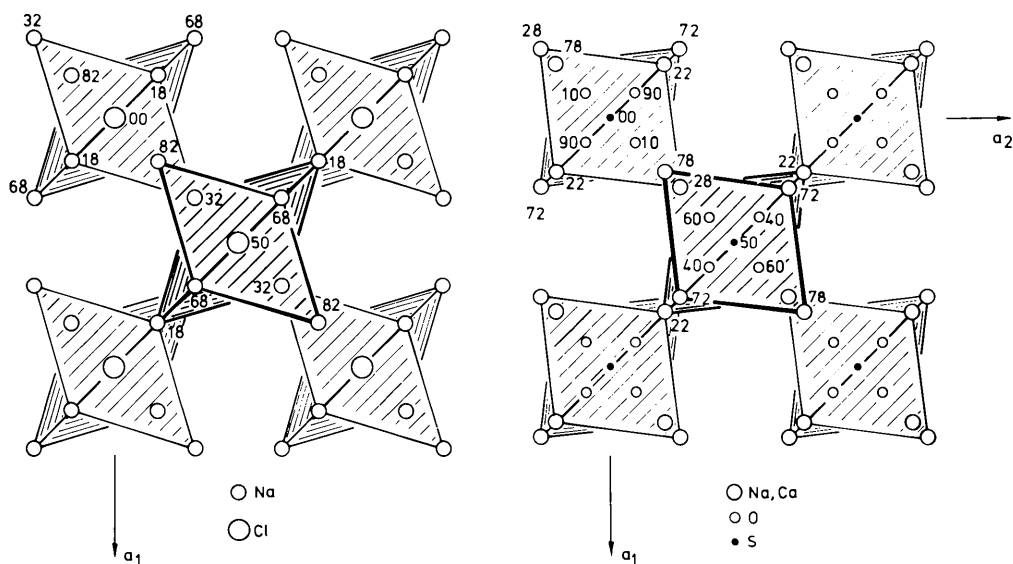


Fig. 9. The framework of *stellae quadrangulae* in sodalite (left) and h a ynite (right).

Table 2. Positions occupied in space groups $Im\bar{3}m$, $I\bar{4}3m$ and $P\bar{4}3n$

<i>Im</i> 3 <i>m</i>						
	2(<i>a</i>)	12(<i>e</i>)	16(<i>f</i>)	24(<i>h</i>)		
Sb_2Ti_7	Tl	Sb	Tl	Tl		
γ -(Mg,Al)	Mg	Al	Al	Mg		
<i>I</i> 43 <i>m</i>						
	2(<i>a</i>)	8(<i>c</i>)	12(<i>d</i>)	12(<i>e</i>)	24(<i>g</i>)	24(<i>g</i>)
α -Mn	Mn	Mn	—	—	Mn	Mn
Ti_3Re_{24}	Ti	Ti	—	—	Re	Re
Zr_5Re_{24}	Zr	Zr	—	—	Re	Re
Er_3Mg_{24}	Er	Er	—	—	Mg	Mg
$Nb_{14.5}Re_{43.5}$	Nb	Nb	—	—	4Nb + 20Re	Re
$Fe_{36}Cr_{12}Mo_{10}$	Mo	Mo	—	—	15Fe + 9Cr	21Fe + 3Cr
$Cr_{17.4}Co_{29.0}Si_{11.6}$	Cr	Cr	—	—	Randomly arranged (Cr,Co,Si)	
$Fe_{40}Re_{18}$ *	Re	Re	—	—	8Re + 16Fe	Fe
Tetrahedrite	S	Sb	Cu	Cu	S	—
Binnite	S	6·8As + 1·2S	Cu	Cu	S	—
<i>P</i> 43 <i>n</i>						
	2(<i>a</i>)	6(<i>c</i>)	6(<i>d</i>)	8(<i>e</i>)	24(<i>i</i>)	
Sodalite	Cl	Al	Si	Na	O	
Hydrosodalite	0·4Cl	Al	5·5Si	7·1Na + 0·7OH	O	
Häüynite	SO ₄	Al	Si	Na,Ca	O	
Helvite	S	Be	Si	Mn,Fe	O	
Na-ultramarine	2·54S	6·08Al	6·35Si	6·86Na	26·2O	
Li-ultramarine	2·11S	6·14Al	5·86Si	4·86Li + 1·68Na	O	
Ag-ultramarine	1·95S	5·8Al	6·2Si	5·25Ag + 2·3Na	O	

* $Fe_{40}Re_{18}$ (Ageev & Sekhtman, 1962).

towards a hexagonal face of the truncated tetrahedron. This arrangement also results in every Cu atom of the SCu_6 octahedra acquiring a triangular S_3 coordination, Fig. 11.

Concluding remarks

By simply varying the rotation angle of the tetrahedral framework to accommodate different sized/shaped

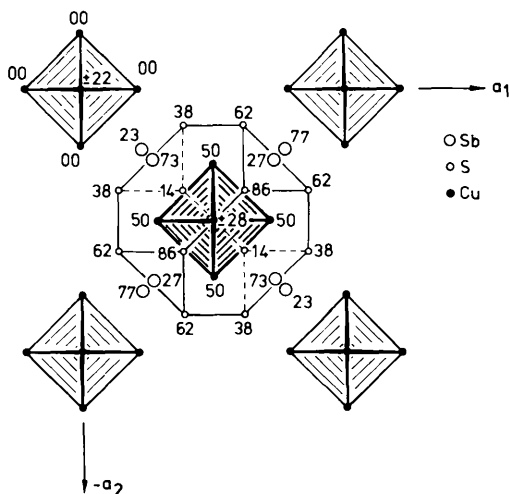


Fig. 10. The interpenetrating part of the structure of tetrahedrite: the SCu_6 octahedra. In the centre a cage in the tetrahedral framework, surrounding the central octahedron, is also outlined.

interpenetrating structures, several different structures can be described. Table 2 lists some of them together with the corresponding occupancy of the different positions of the structure. Position 12(*d*) of $I43m$, which is split into the two sixfold positions 6(*c*) and 6(*d*) in $P43n$, centres the tetrahedra forming the framework. It is unoccupied in the alloy structures.

A similar rotation mechanism, but with a framework of different topology, was recently used for obtaining families of structures related to cristobalites (O'Keeffe & Hyde, 1976).

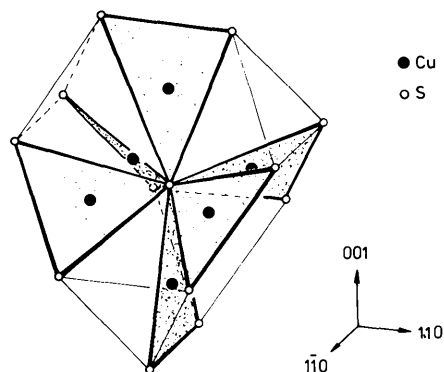


Fig. 11. A clinographic projection of the central part of the tetrahedrite structure shown in Fig. 10. The triangular S-atom coordination around every Cu atom is shown.

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Colour Lattices and Spin Translation Groups. General Case*

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Abstract

A method of deriving d -dimensional crystallographic colour lattices with no symmetry conditions on the basis vectors is given. A number of nonequivalent n -colour lattices is evaluated for $d \leq 4$ and any finite n . An application of colour lattices for obtaining spin translation groups is presented. The results for triclinic spin translation groups are compared with those of Litvin [*Acta Cryst.* (1973), **A29**, 651–660].

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1. Introduction

Colour groups in crystallography are defined as extensions of classical crystallographic groups. The idea started in the works of Below & Tarkhova (1956), Indenbom (1959), Niggli (1959) and others (see also Shubnikov & Koptsik, 1974). Colour groups are of interest in the theory of magnetic crystals, alloys, defect crystals, etc. Magnetic groups have been interpreted in terms of two-colour groups. The generalized magnetic groups called spin groups have been recently introduced in the form of many-coloured groups.

Different types of colour groups, their properties and bibliography have been reviewed by Shubnikov & Koptsik (1974) and Opechowski (1977). Only P -type colour groups will be considered here. Colour point groups have been derived by Koptsik & Kotsev (1974a) and Harker (1976). Zamorzaev (1969),