

The Packing Analogues of Sodalite, Tetrahedrite and Related Structures*,#

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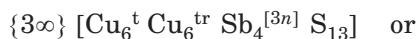
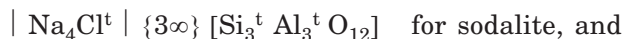
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Sodalite and tetrahedrite are normally treated separately because they are chemically very different and do not appear to be related. However, if appropriate representations (packing analogues) are used, one can realise how similar they are in crystal structure. Other interesting relationships, though not so close, may also be found with cristobalite and MgCu_2 (Friauf-Laves phase).

Key words: sodalite, tetrahedrite, packing analogues, structure relationships.

Sodalite (chlorine sodium aluminosilicate) and tetrahedrite (copper antimony sulphide) are both framework structures, and their corresponding structural formulae are:



* Dedicated to Professor Boris Kamenar on the occasion of his 70th birthday.

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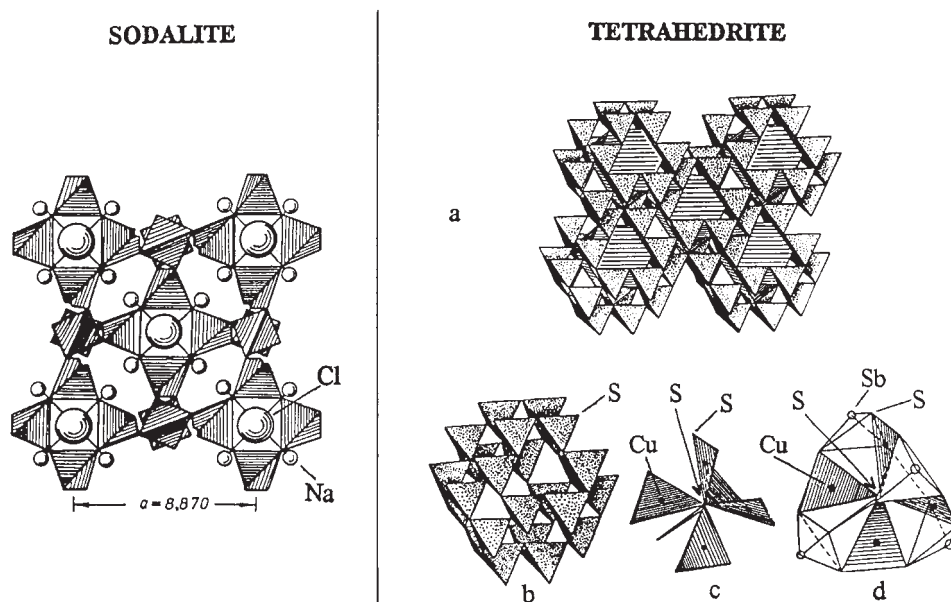
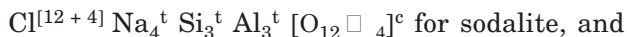


Figure 1. The sodalite framework projected on (100) (adapted from Povarennykh, 1972),¹ and (a) the tetrahedrite framework of CuS_4 tetrahedra; (b) spatial arrangement of the CuS_4 tetrahedra showing the large cage (truncated tetrahedron); (c) triangular coordination, tr, of Cu; (d) complete coordination [12 + 4 + 6] of certain sulphur atoms (adapted from Povarennykh, 1972).¹

Their structures appear quite different on Figure 1, and they show an odd coordination for certain atoms.

Let us consider the packing analogues of these minerals. The packing analogue of a certain structure is the close-packed structure which is structurally very similar to it (Figueiredo 1977, Lima-de-Faria, 1988, 1994).²⁻⁴ An example is diopside and its packing analogue cobalt germanate.

Tetrahedrite has also been described as a defect substitution derivative of sphalerite, ZnS , and is therefore based on a defect cubic closest packing of the sulphur atoms with copper and antimony in tetrahedral interstices. Sodalite can be considered as a defect cubic closest packing of the oxygens, with silicon and aluminium occupying the tetrahedral voids. Structural formulae of their packing analogues are:



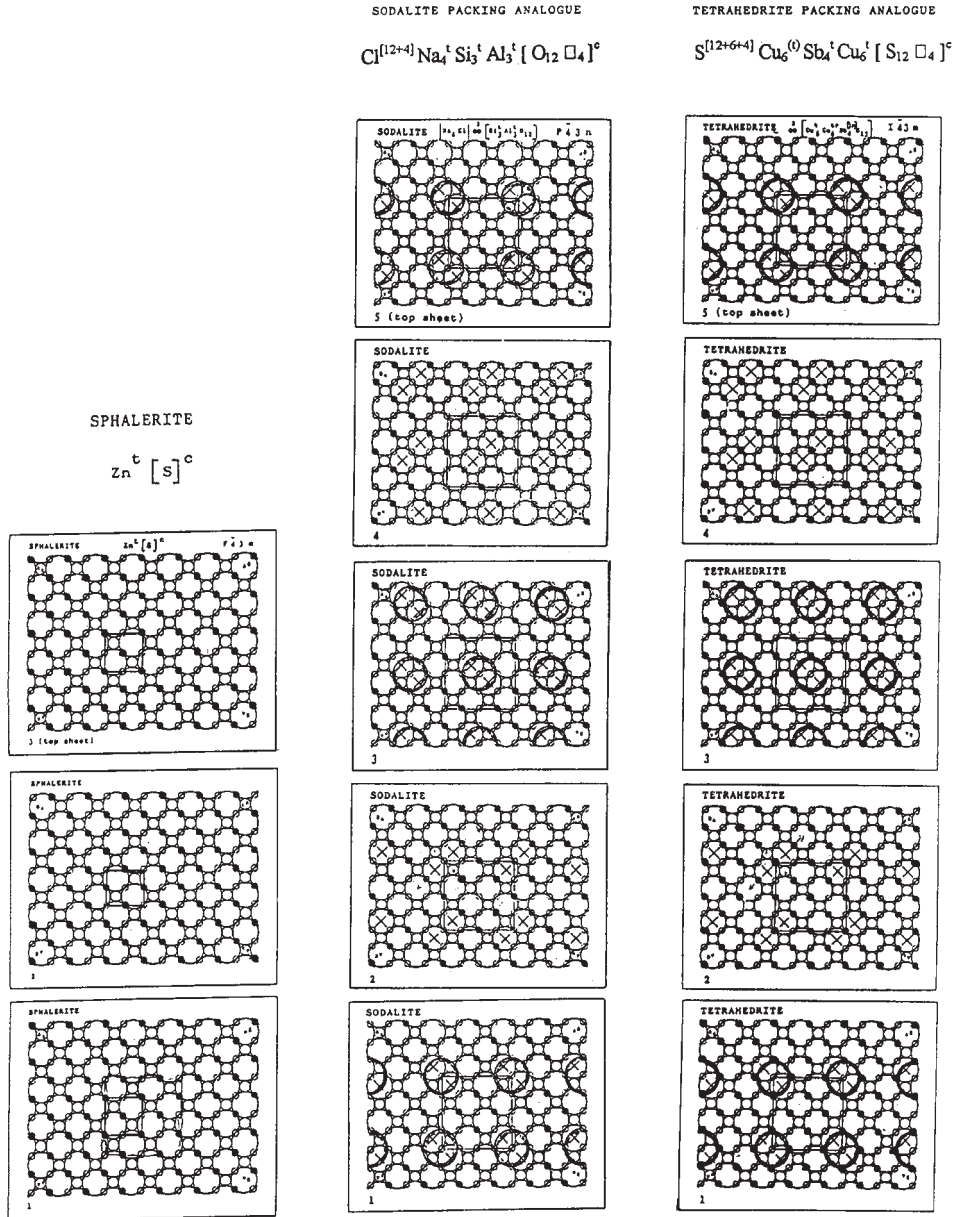
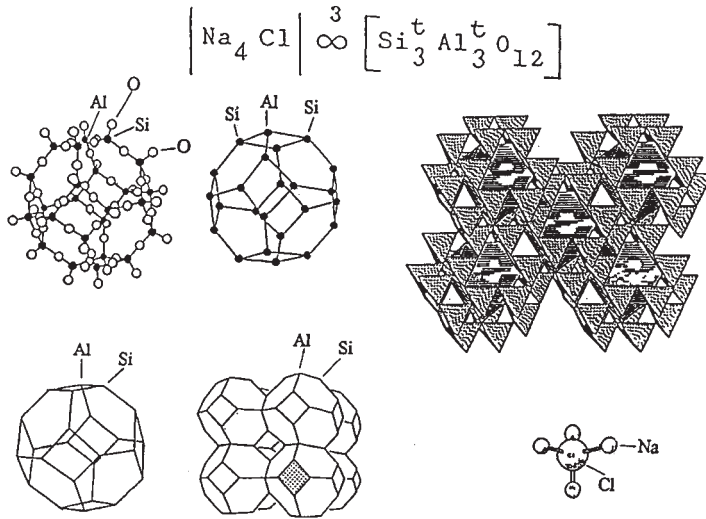


Figure 2. Condensed models of sphalerite, and of the sodalite and tetrahedrite packing analogues. The crosses represent missing packing atoms, the small circles the atoms in tetrahedral coordination, and the larger circles the atoms that fit in the cages (certain S atoms, in the case of tetrahedrite, and Cl atoms in sodalite).

SODALITE

 $P\bar{4}3n$ 

TETRAHEDRITE

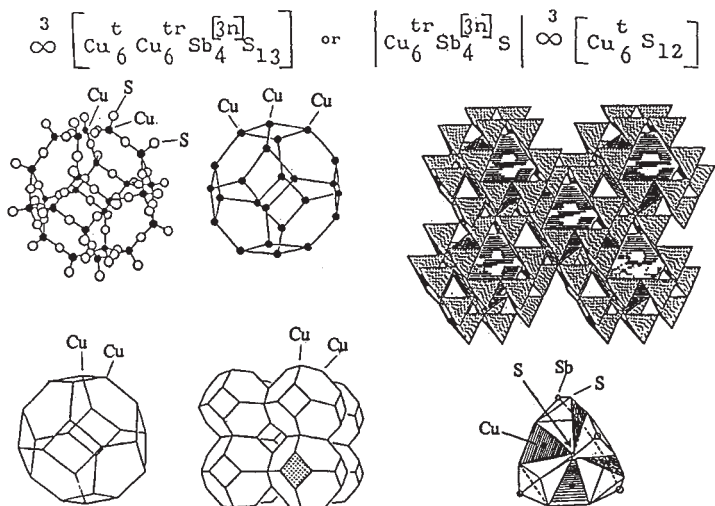
 $I\bar{4}3m$ 

Figure 3. Sodalite framework of $(\text{Si,Al})\text{O}_4$ tetrahedra (adapted from Belov, 1963), and details of the structure.⁵ Tetrahedrite framework of CuS_4 tetrahedra, and details of the structure.

where (t) means tetrahedral coordination regardless of the deficiency. The corresponding condensed models are presented in Figure 2. This relationship between the two structures demonstrates their similarity (Figure 3).

Some structures based on defect close packing may exhibit odd coordination of the interstitial atoms, as in the case of certain sulphur atoms in tetrahedrite, $CN = 12 + 4 + 6$. The existence of the unusual coordination is explained; some of the close-packed atoms are missing. (Sphere packing models may help to elucidate the coordination.)

Other structures, which apparently seem unrelated to sodalite and tetrahedrite, are $MgCu_2$ (a Friauf-Laves phase) and SiO_2 , cristobalite. The $MgCu_2$ is a close-packed structure formed by a mixed packing (heterogeneous packing) of Mg (large) and Cu (small) atoms. Cristobalite is a framework structure of SiO_4 tetrahedra. Both structures can be imagined as being built of defect cubic closest packing of Cu atoms in the case of $MgCu_2$, and of O atoms in cristobalite. In these two structures the packing is more defective, but the missing crossed pairs of packing atoms give rise to the same cages (truncated tetrahedron) as in the sodalite and tetrahedrite structures. In the Friauf-Laves phase $MgCu_2$, large Mg atoms occupy these cages; in cristobalite the cages are unoccupied.

The use of structural formulae and of various kinds of crystal structure representation, including packing analogues whenever possible, is strongly recommended in order to help understanding the relationship among structures.

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SAŽETAK**Analozi sodalita, tetrahedrita i srodnih struktura po pakovanju***Jose Lima-de-Faria*

S obzirom na bitnu razliku u kemijskom sastavu i činjenicu da se ne doimlju srodnim, strukture sodalita i tetrahedrita obično se ne uspoređuju. Međutim, ako se rabe primjereni prikazi slagalina atoma svatko može vrlo lako uočiti kako su kristalne strukture tih minerala slične. Zanimljivi suodnos, premda ne tako blizak, može se također zamijetiti između kristobalita i MgCu_2 (Friauf-Lavesova faza).