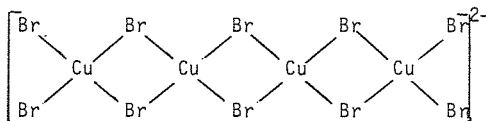


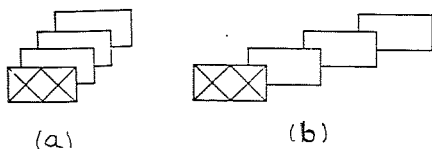
08.1-7 THE CRYSTAL STRUCTURE OF $[(CH_3)_3NH]_2Cu_4Br_{10}$:
 STACKING PATTERNS OF QUASI-PLANAR BIBRIDGED $Cu_nX_{2n+2}^{2-}$
 AND $Cu_nX_{2n}^{2-}$ OLIGOMERS. By Roger D. Willett and Urs
 Geiser, Department of Chemistry, Washington State Uni-
 versity, Pullman, WA 99164-4630 USA.

The title compound crystallizes in the monoclinic space
 group $P2_1/a$ with $a = 19.054(9)A$, $b = 14.719(7)A$,
 $c = 9.566(3)A$, and $\beta = 109.87(3)^\circ$. The compound con-
 tains nearly planar bibridged $Cu_4Br_{10}^{2-}$ anions with
 Cu-Br distances of 2.3-2.5A and bridging Cu-Br-Cu
 angles from 93° to 96° . In addition to the four normal



Cu-Br bonds, each copper forms one or two additional
 semi-coordinate Cu-Br bonds, yielding a final 4 + 1
 or 4 + 2 coordination geometry, and forming chains
 parallel to the c axis. Although an analogous tetramer
 exists in the corresponding chloride salt, the stacking
 of the tetramers is different. In the latter, a uni-
 form stacking arrangement is attained, with three of
 the four copper ions forming long Cu-Cl bonds to chlor-
 ide ions in neighboring units. For the bromide salt,
 the bromide ions alternately cover three and four
 copper ions in adjacent tetramers.

We introduce a notation where we specify the relative
 displacement of adjacent oligomers in terms of the
 ligand-ligand distance, d , along the edges. It is
 necessary to specify both the translation parallel
 ($n_{||}d$) and perpendicular ($n_{\perp}d$) to the Cu-Cu direction,
 yielding a vector notation, $(n_{||}, n_{\perp})$. Thus the dimer
 stacking in (a) is specified by $(1/2, 1/2)$, while that
 in (b) is given by $(3/2, 1/2)$.



As another example, the stack of $Cu_3Br_8^{2-}$ trimers in
 $[(C_2H_5)_2NH]_2Cu_4Br_{10} \cdot C_2H_5OH$ is given by the pair of
 vectors $(1/2, 1/2)(-1/2, -1/2)$ - e.g. - alternate
 trimers stack exactly on top of each other.

In this notation, the uniform stacking in
 $[(CH_3)_3NH]_2Cu_4Cl_{10}$ is given by $(3/2, 1/2)$ while the
 alternate stacking in the title compound is specified
 by the pair $(3/2, 1/2)(1/2, -1/2)$.

08.1-8 KRISTALLPACKUNG IN EPh_4^+ -SALZEN.
 Ulrich Müller, Fachbereich Chemie der Universi-
 tät, Hans-Meerwein-Str., D-3550 Marburg,
 Deutschland.

Verbindungen $EPh_4^+X^-$ ($E = P, As$; $X^- =$ anorgani-
 sches Anion) kristallisieren häufig unter Aus-
 bildung von Säulen aus übereinandergestapelten
 EPh_4^+ -Ionen. Die EPh_4^+ -Ionen erfüllen exakt oder
 näherungsweise die Symmetrie 4. Je nach Symme-
 trie des Anions ist die Raumgruppe $P4/n$ oder
 $I4$ oder eine Untergruppe davon. Beispiel:
 $PPh_4MoOCl_4 (P4/n) \text{ --- } PPh_4ReCl_4N_2S_2 (P2/n) \text{ --- } PPh_4SnCl_3 (P1)$.

In Verbindungen $(EPh_4^+)_2X^{2-}$ ordnen sich je zwei
 EPh_4^+ -Ionen um ein Inversionszentrum, indem drei
 Phenylgruppen des einen Ions in die Lücken zwis-
 chen drei Phenylgruppen des anderen ragen. Die
 $(EPh_4^+)_2$ -Paare können zu Stäben aneinandergereiht
 sein, die parallel gebündelt sind (Typ I), oder
 es werden Schichten gebildet. Die Schichten
 sind entweder unmittelbar aufeinander gestapelt
 (Typ II) oder zwischen ihnen befinden sich wei-
 tere $(EPh_4^+)_2$ -Einzelpaare (Typ III). Dabei blei-
 ben in jedem Fall Hohlräume, welche die Anionen
 aufnehmen. Beispiel: $(AsPh_4)_2UCl_6 \cdot 2 CH_2Cl_2$ mit
 zwei Modifikationen vom Typ I und III.

08.1-9 A STRUCTURE CLASSIFICATION OF CONDENSED MODES
 IN ABX_4 COMPOUNDS. By R. Deblieck, J. Van Landuyt and S.
 Amelinckx. Universiteit Antwerpen, RUCA, Groenenborger-
 laan 171, B-2020 Antwerp, Belgium.

Some ABX_3 (perovskite) compounds such as $CaTiO_3$ and
 $NaNbO_3$ undergo phase transitions due to the condensation
 of soft phonons. The structure of the lower temperature
 phase can be described in terms of the tilting of the BX_6
 octahedra around one or some of their tetrad axes.
 Glazer (Acta Cryst. (1972). B28, 3384), classified these
 structures in tilting schemes using the correlation of
 tilting of the octahedra along the "pseudocubic" axes
 connecting the B-cations at right angles.

In ABX_4 -compounds, although the octahedra are not vertex-
 shared in the third dimension, phase transitions involving
 soft modes do occur also (M. Hidaka et al., J.Phys.C.Sol.
 St. Phys. (1979). 12, 2737; J.Phys.C.Sol.St.Phys. (1979). 12,
 1799; Phys. stat.sol. (a) (1982). 72, 809).

Consequently Glazers' classification was extensively used
 for the description of the structures of the lower temper-
 ature phases of ABX_4 -compounds as well.

It is however quite obvious that this description will be
 degenerate when applied to ABX_4 compounds, because of the
 supplementary degrees of freedom present in these com-
 pounds: i.e. when a particular tilting scheme has been
 applied consistently to two successive layers of vertex-
 shared octahedra these layers may still be shifted rel-
 ative to one another over a vector \vec{R} with four distinct
 possibilities: $\vec{R} = (0,0)$; $\vec{R} = (a,0)$; $\vec{R} = (0,b)$;
 $\vec{R} = (a,b)$, yielding possible new structures.

It is our aim to present a similar non degenerate classi-
 fication whereby an exhaustive count is made of all
 possible structures in the ABX_4 -case, including a sche-
 matical representation of the structure and a structure
 factor calculation of all relevant reflections for each
 possible structure.