

05.2-12 THE CRYSTAL STRUCTURES OF QUASI ONE-DIMENSIONAL CONDUCTORS ON THE BASE OF TETRATHIOTETRACENE (TTT) AND TETRASELEMO-TETRACENE (TSeT) WITH INORGANIC ANIONS. By R.P.Shibaeva and V.F.Kaminskii, Institute of Chemical Physics, USSR Academy of Sciences, 142 432 Chernogolovka, U.S.S.R.

We have carried out the X-ray analyses of the new cation-radical salts such as TTT^+Br^- , $\text{TTT}^+(\text{CuBr}_2)^-$, $\text{TSeT}^+(\text{CuBr}_2)^-$, $\text{TTT}_3^{2+}(\text{Hg}_2\text{Br}_6)^{2-}$ and also the cation-radical salts formed in the reaction of TTT (TSeT) with HgX_2 (X=I, Br, Cl) [1-3]. Some of these salts have rather high values of conductivity at room temperature, $\sigma \sim 10^3 \text{ ohm}^{-1}\text{cm}^{-1}$. As distinct from the isostructural complexes $\text{TTT}\cdot\text{TCNQ}_2$ and $\text{TSeT}\cdot\text{TCNQ}_2$ the crystals $\text{TTT}^+(\text{CuBr}_2)^-$ and $\text{TSeT}^+(\text{CuBr}_2)^-$ are not isostructural. The important feature of $\text{TTT}\cdot\text{CuBr}_2$ structure is the presence of cation-radical stacks with the alternate interplanar TTT-TTT spacings of 3.24 and 3.63 Å. The anion in this structure is in the form of a centro-symmetrical dimer $(\text{Cu}_2\text{Br}_4)^{2-}$. The existence of segregate regular stacks of TSeT^+ with interplanar distance of 3.55 Å is characteristic of $\text{TSeT}\cdot\text{CuBr}_2$ structure. The anion of this complex has a strongly distorted linear configuration with Br-Cu-Br angle of 154.7°. $\text{TTT}_3(\text{Hg}_2\text{Br}_6)$ crystals are isostructural with $\text{TTT}_3(\text{Hg}_2\text{Cl}_6)$, and those of $\text{TSeT}_3(\text{Hg}_2\text{Cl}_6)$ with $\text{TSeT}_3(\text{Hg}_2\text{Br}_6)$ crystals.

The comparison of the geometry of the TTT^+ , TSeT^+ -cation-radicals and TTT, TSeT neutral molecules is given on the basis of X-ray crystallographic data. In particular, it is shown that the bond lengths Se-Se, S-S and Se-C, S-C in cation-radicals are shorter than in neutral molecules. The crystal structures and electrical properties of the salts in question and all presently well known organic quasi one-dimensional conductors on the basis of TTT and TSeT are analyzed.

- [1] R.P.Shibaeva, V.F.Kaminskii, N.D.Kushch, A.V.Zvarykina, E.B.Yagubskii, Dokl.Acad. Nauk SSSR, 251, 162 (1980)
- [2] R.P.Shibaeva, V.F.Kaminskii, O.N.Eryemenko, E.B.Yagubskii, M.L.Khidekel. Kristallografiya, 25, 60 (1980)
- [3] R.P.Shibaeva, V.F.Kaminskii. Kristallografiya, 26, 332 (1981).

05.2-13 THE ROLE OF STRUCTURE ON SUPERCONDUCTIVITY OF A15-SUPERCONDUCTORS.

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A15-compounds have been known to have by far the most favourable structure for the occurrence of superconductivity.

The relationship between the superconducting transition temperature (T_C) and the number of electrons/atom as well as cell constants will be discussed. (B.T. Matthias, Phys.Rev. (1953) 92, 874; D.U.Gubser, H.R.Ott & K.Girgis, Phys.Rev. (1979) B19, 199). Further, the long range order (LRO) and T_C dependence will be treated in detail. The LRO parameter is dependent on heat treatment and stoichiometry and is greatly affected by neutron and ion bombardment. Clarification of discrepancies and contradictions in the literature will be attempted (E.C.Blaugher et al., J. Low Temp.Phys. (1969) 1, 539; F.E.Wang & J.R. Holden, Solid State Commun. (1974) 14, 443).

The typical and atypical A15-compounds and their structure differences will be explained (H.L. Staudenmann, Thesis No. 1735 (1976) Genève; K.Girgis & P.Fischer, Neutron Streuung Progr. Rep. (1974) 80, 59; etc.).

And last: how can the max. T_C -values be reached?

A review of the literature and our own results will be presented.

05.2-14 PREMARTENSITIC STATES IN ORDERED

$\text{Cu}_{68}\text{-Zn}_{15}\text{-Al}_{17}$ ALLOY. By A.A. Katsnelson and N.A. Khatanova. Faculty of physics, Moscow State University, Moscow, USSR.

Studies of crystal structure of quenched $\text{Cu}_{68}\text{-Zn}_{15}\text{-Al}_{17}$ alloy employing electron diffraction show that a type of martensitic structure depends on solid solution ordering. If the solid solution is ordered according to Fe_3Al (DO_3) type, then M18R martensite is formed (Chakravorty, Wayman, Acta Met. (1977) 25, 989). If the ordering is of CsCl(B2) type, then in the same alloy 2H martensite with a distorted structure is formed. The formation of different martensites in this alloy is the result of different acoustic phonon's "softening", which takes place prior to the martensitic transformation. At this stage electron diffraction study shows the existence of short diffuse streaks, passing through the matrix' reflections. If the matrix is ordered like DO_3 , the streaks run along $\langle 110 \rangle^*$, but if the ordering is like B2 - the streaks run along $\langle 112 \rangle^*$. These streaks can be caused by "softening" of different acoustic phonons' modes in DO_3 and B2 solid solution before the transformation. We believe that DO_3 - M18R transition begins with "softening" of $\{110\}\langle 110 \rangle$ acoustic mode, while B2 - 2H transition needs the "softening" of $\{112\}\langle 111 \rangle$ acoustic mode.