

12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

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defect structures are only metastable which is important for the long time use of these materials.

In spite of a lower concentration of vacancies (tetragonal) Y-TZP ($Zr_{1-2x}Y_{2x}O_{2-x}$ with $x \approx 0.03$) shows superior conductivity at temperatures below 1000 K, roughly. This is related to a more random distribution of the defects. In addition, the diffusion pathways as determined from pdf-maps differ appreciably in both materials being slightly more favourable in TZP (where they are restricted to certain double layers) mainly due to the more favourable arrangement of the atoms in the tetragonal structure. The conductivity can be further enhanced by alloying with Ti or Ce which may again be related to an increasing "tetragonality" (c/a ratio, $z(O)$ parameter).

Although similarities with zirconia are present in ceria ($Ce_{1-2x}Y_{2x}O_{2+x}$, $0 \leq x \leq 0.1$) the disorder is more complex as evidenced by additional weak superlattice peaks which may be assigned to certain substoichiometric phases CeO_{2-y} . Moreover, the disorder depends on preparation conditions and changes with temperature.

In $LiNbO_3$ (and isotypic $LiTaO_3$) deviations from stoichiometry occur without alloying with other atom species. New structure refinements disagree with previously reported disorder models: no vacancies on the Nb lattice, excess Nb on Li sites with corresponding Li vacancies. At high temperatures Li becomes mobile leading to an order-disorder phase transition at 1480 K. Diffuse planes perpendicular to (-221) are assigned to uncorrelated Nb-O-Nb chains as identified from a static contribution to the corresponding temperature factors. Intensity concentrations at low temperatures (25 K) indicate the onset of short range order correlations.

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DS-12.02.05 Diffuse Scattering from the Organic Conductor $C_1TET - TTF.(AuI_2)_{2/3}$.

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The sample is electrochemically prepared with a constant current of $25 \mu A$ at $25^\circ C$ in a 1,1,1-trichloroethane/ acetonitrile solution of $C_1TET - TTF$ (Bis(methylthio)ethylenedithio-TTF, a hybrid molecule between $BEDT - TTF$ and $TTC_1 - TTF$) and tetrabutylammoniumdiiodoaurate. The crystals are very brittle little black bars.

X-ray diffraction intensity data of a single crystal of $C_1TET - TTF.(AuI_2)_{2/3}$ were collected with graphite monochromatized radiation on an Enraf Nonius CAD4F diffractometer, all reflections with h odd being weak. The spacegroup is $P2_1/c$ with $a = 7.54 \text{ \AA}$, $b = 22.45 \text{ \AA}$, $c = 11.67 \text{ \AA}$, $\beta = 100.14^\circ$, $V = 1945.2 \text{ \AA}^3$ and $Z = 4$, one unit being $C_{10}H_{10}S_8(AuI_2)_{2/3}$. The structure was solved and refined with DIRDIF and Xtal 3.0 software packages. Final conventional refinement gives $R = 0.065$, $wR = 0.055$ and $S = 2.988$.

The structure consists of ordered organic residuals forming zigzag layers parallel (100), leaving channels along [100] and disordered gold-iodine chains within these channels. In the average structure the disorder shows up as very large temperature factor parameters of gold and iodine in the chain direction, fractional occupation numbers and unphysical distances between peak positions ($\approx 1 \text{ \AA}$). Rotation photographs on a Weissenberg camera show diffuse planes perpendicular to the a -axis with h -indices 0.8, 1.6, 2.4 and 3.2. The planes consist of diffuse peaks superimposed on slowly varying greyness. The diffuse scattering can be explained by a tentative model with independent chains of four (AuI_2^-) -ions per five times the a -axis length. More results will be presented in detail.

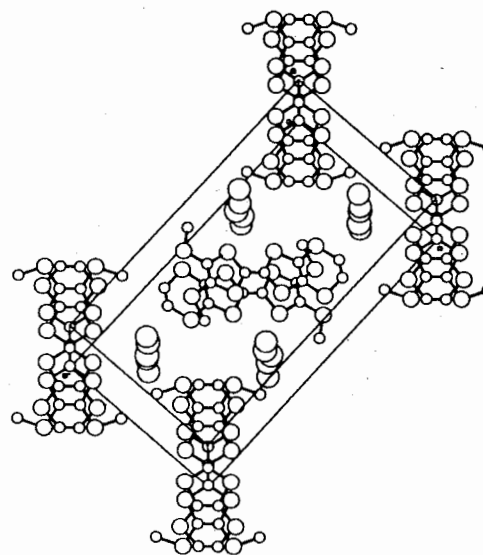


Fig. 1. The structure of $C_1TET - TTF.(AuI_2)_{2/3}$.

DS-12.02.06 X-RAY DIFFUSE SCATTERING STUDY OF DISORDERS IN ORGANIC CONDUCTORS AND SUPERCONDUCTORS by J.P. Pouget*, Laboratoire de Physique des Solides (CNRS UA2), Université de Paris Sud, 91405 ORSAY, France

Electronic and structural properties as well as instabilities exhibited by quasi one dimensional (1D) conductors are very sensitive to disorders such as those created by irradiation or substitution. Disorder in particular induces electronic localization, suppresses the superconductivity and pins the $2k_F$ spin and charge density wave (SDW and CDW respectively) modulations (k_F is the Fermi wave vector of the 1D electron gas). In spite of these dramatic effects there is only very few detailed studies of the structural modifications induced by the disorders in the different families of low dimensional organic conductors and superconductors.

Substitutional and orientational disorders present in the family of quasi-1D organic superconductors $(TMTSF)_2X$ based on the tetramethyltetraselenafulvalene molecule and where X is monovalent anion like PF_6 , ReO_4 have been characterized by simulations of their X-ray diffuse scattering