DS-12.02.05 Diffuse Scattering from the Organic Conductor Cu$_3$TET – TTF·(AuI$_2$)$_{1/2}$

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The sample is electrochemically prepared with a constant current of 20 mA at 25°C in a 1,1,1-trichloroethane/acetonitrile solution of Cu$_3$TET – TTF·(AuI$_2$)$_{1/2}$. Cu Kα $\alpha$-monochromatized radiation was recorded with Enraf Nonius CAD4 diffractometer, all reflections with $h$ odd being weak. The spacegroup is $P2_1/c$ with $a = 7.54\AA$, $b = 22.43\AA$, $c = 11.67\AA$, $\beta = 100.14°$, $V = 1945.2\AA^3$ and $Z = 4$, one unit cell = Cu$_3$Hfi$_2$(AuI$_2$)$_{1/2}$. The structure was solved and refined with Diffrac and Xsal 3.0 software packages. Final conformation refinement gives $R = 0.06$, $wR = 0.065$ and $S = 2.08$.

DS-12.02.06 X-RAY DIFFUSE SCATTERING STUDY OF DISORDERS IN ORGANIC CONDUCTORS AND SUPERCONDUCTORS by J.F. Pouget, Laboratoire de Physique des Solides (CNRS URA 249, 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 disorder such as those created by irradiation or substitution. Disorder in particular induces electronic localization, suppresses the superconductivity and pins the 2$p$ spin and charge density wave (SDW and CDW respectively) modulations (kp is the Fermi wave vector of the 1D electron gas). In spite of these dynamic 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)$_2$X 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.

Fig. 1. The structure of Cu$_3$TET – TTF·(AuI$_2$)$_{1/2}$.
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pattern. It is found that in most of the cases the disorder is random but accompanied by molecular displacements (size effect). Its consequences on the various instabilities by these defects will be discussed. In particular those involving the ordering of non-centrosymmetric units will be interpreted in term of random interactions or random fields due to the disorder. Incommensurate 2k SDW and 2k CDW modulations observed in many quasi 1D conductors can collectively slide under the action of an external electric field when its intensity overcomes a threshold value due to the pinning of the waves to defects. The microscopic mechanism of this pinning mechanism is up to now poorly documented. Very recently we have succeeded to observe in the TTF-TCNQ family of charge transfer salts disordered by irradiation or substitution, asymmetric X-ray diffuse scattering effects allowing to determine the phase of the CDW as well as its spatial variation, in the vicinity of the defects. This work has been done in collaboration with V.LAKOVAC, Q LIU and S.RAY. It has been partly supported by the CEC ESPRT – Basic Research Action MOLCOM 3121.

PS-12.02.08 FULLERENES AND THE STRUCTURE OF CARBONS
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The discovery of the cage-like molecular allotropic form of carbon, the fullerenes, in particular C_{60} ("buckminsterfullerene"), has been extensively documented (W. S. Kroto, Angew. Chem. Int. Ed. Engl., 1992, 31, 111-129). In C_{60} it was postulated that a carbon atom is located at each vertex of a truncated icosahedron. This structure was subsequently confirmed in single crystal and powder preparations variously using spectroscopy and diffraction (W. Krätschmer et al., Nature, 1990, 347, 355-358; W. L. F. David et al., Nature, 1991, 355, 147-154).

The possible role of the fullerences in the constitution of carbon and non-graphitic carbons is considered in the context of (a) several recent studies, (b) the conclusions drawn in earlier investigations on carbons, including the anticipation of cage-like structures by J. Gibson, M. Helman, and H. L. Tielay (J. Chem. Soc. Lond., 1946, Part 1, 456-461), and (c) the way in which we may now interpret some of R. A. Frankland’s very detailed analyses of carbons (Acta Cyst., 1990, 3, 107-107).

PS-12.02.09 STRUCTURAL STUDY OF AMMINE GROUP IN Ni(NH3)4Cl2 BY X-RAY DIFFRACTION. By M. Shiono*, Y. Yarin, N. Achiwa, Department of Physics, Kyushu University, Higashi-ku, Fukuoka, Japan and N. Koyano, Research Reacto Institute, Kyoto University, Kumatori, Osaka, Japan.

Crystals of Hexa-ammine Metal complexes are commonly known to have disordered structures due to the rotational motions of the ammonium molecules. We have analyzed the electron density distributions of hydrogen atoms in Ni(NH3)4Cl2 single crystal (space group Fm3m, a = 10.080(1)Å) by x-ray diffraction. Difference Fourier synthesis is used in order to classify the density of hydrogen atoms. Data were collected with 4-circle diffractometer, Rigaku AFC5R. Monochromatized Mo Kα radiation was used. The total number of reflections measured was 3699 (sinθ/λ = 1.09Å⁻¹). Averaging procedure gave 328 independent reflections. Least-squares refinement and D-synthesis were performed with 145 reflections (F ≥ 3σ(F)).

The D-Fourier map of the hydrogen density is shown in Fig.1. The square figure with a peak at the each corner is comparable with the neutron-diffraction result of Ni(NH3)4H2O (Iosser, A., Prandi, W., Schiebel, P., and Beger, G. (1989) Physica B. 158-157, 85-87). The map in (001) plane is shown in Fig.2. Cross sections of the hydrogen density are clearly seen. In addition, density of lone pairs of nitrogens appears across the triangular craters from the hydrogen density.