

## 10-Physical and Chemical Properties of Materials in Relation to Structure (Superconductors, Fullerenes, etc)

K (Dyachenko, O.A., Gritsenko, V.V., Mkyan, Sh.G., Shilov, G.V., & Atovmyan, L.O. *Izv. AN SSSR. Ser. Khim.*, 1991, 2062-2070),  $(\text{ET})_8[\text{Hg}_4\text{Cl}_{12}(\text{PhBr})_2]$  (6) which is metallic to 10 K,  $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{PhCl})_2]$  (7) with  $T_{\text{MI}} = 90$  K,  $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{PhBr})_2]$  (8) with  $T_{\text{MI}} = 125$  K (Gritsenko V.V., Dyachenko, O.A., Shilov, G.V., Lyubovskaya, R.N., Afanasyeva, T.V., Lyubovskii, R.B. & Makova, M.K. *Izv. AN. Ser. Khim.*, 1992, 894-902),  $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{MePhCl})_2]$  (9),  $(\text{ET})_4[\text{Hg}_3\text{I}_8]$  (10) (Takhirov, T.G., Krasochka, O.N., Dyachenko, O.A., Atovmyan, L.O., Aldoshina, M.Z., Goldenberg, L.M., Lyubovskaya, R.N., Merzhanov, V.A. & Lyubovskii, R.B. *Mol. Cryst. Liq. Cryst.*, 1990, 185, 215-226),  $(\text{ET})_4[\text{Hg}_2\text{I}_6]$  (11),  $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Cl}]$  (12) with  $T_{\text{MI}} = 50$  K (Konvalikhin, S.V., Shilov, G.V., Dyachenko, O.A., Lyubovskaya, R.N., Aldoshina, M.Z. & Lyubovskii, R.B. *Izv. AN. Ser. Khim.*, 1992, 903-909),  $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Br}]$  (13) with  $T_{\text{MI}} = 140$  K,  $(\text{ET})_2[\text{Hg}(\text{SCN})\text{Cl}_2]$  (14) with  $T_{\text{MI}} = 35$  K (Konvalikhin, S.V., Shilov, G.V., Dyachenko, O.A., Aldoshina, M.Z., Lyubovskaya, R.N. & Lyubovskii, R.B. *Izv. AN. Ser. Khim.*, 1992, 2323-2331),  $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Br}_{0.66}\text{Cl}_{0.33}]$  (15) with  $T_{\text{MI}} = 70$  K and  $(\text{d}_8\text{-ET})_4[\text{Hg}_2(\text{SCN})_4\text{Cl}_2]$  (16) with  $T_{\text{MI}} = 86$  K. The named compounds are characterized by a variety of electroconducting properties including superconductors (1-4), metals (5-8, 12-16) and semiconductors (9-11). As a result of a comparative study of the crystal structures of the compounds (1-16) and organic conductors related to them, a variety of the types of ET packing in the conducting layers and the anion structures have been shown. The factors affecting the structural design and electroconducting properties of the organic conductors and superconductors are discussed.

### 10.02 - Fullerenes

MS-10.02.01 SYNCHROTRON X-RAY STUDY OF THE ORIENTATIONAL ORDERING IN SINGLE CRYSTAL  $\text{C}_{60}$ . By P. Wochner, P. C. Chow, G. Reiter, S. C. Moss, University of Houston, Houston, TX 77204-5506 USA; J. D. Axe, J. C. Hanson, R. K. McMullan, Brookhaven National Laboratory, Upton, NY 11973 USA; P. Zschack, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA; M. C. Nelson, University of Illinois, Urbana, IL 61801 USA.

The determination of both the single molecule and intermolecular interaction potentials provides a key to the understanding of the orientational ordering transition at 260K. These potentials can be extracted, respectively, from Bragg (P. C. Chow et al., *Phys. Rev. Lett.*, 1992, 69, 2943-2946) and diffuse X-ray scattering experiments which probe the orientational pair correlations between  $\text{C}_{60}$  molecules as a function of their separation (J. R. D. Copley and K. H. Michel (preprint)). We will show that even in the orientationally disordered state, with continuously re-orienting  $\text{C}_{60}$  molecules, a given molecule will show preferential orientation resulting in deviations from a spherical distribution. These deviations allow us to evaluate the probability of orientation

$P(\tilde{\omega})$  and the effective single molecule potential energy  $V(\tilde{\omega})$ , where  $\tilde{\omega}$  is the set of Euler angles.

In a large single crystal, grown by J. Z. Liu and colleagues at UC Davis, we have observed anisotropic zone boundary diffuse scattering, extending well above the first-order transition temperature  $T_c$ , which is strongly dependent on the scattering wave vector,  $\tilde{Q}$ . This scattering is associated with the form factor variation for a single molecule in the crystal field, which is then modulated by the scattering from coherent orientational correlations. We will present current progress in our determination of the interaction potential.

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MS-10.02.02 CRYSTAL STRUCTURES OF  $\text{C}_{60}$  AND OF  $(\text{HYDROQUINONE})_3\text{C}_{60}$ . By H.-B. Bürgi and M. Foertsch, Laboratory of Crystallography, University of Bern, Switzerland; R. Restori and D. Schwarzenbach\*, Institute of Crystallography, University of Lausanne, Switzerland; O. Ermer, Institute of Organic Chemistry, University of Köln, Germany.

Pure  $\text{C}_{60}$  undergoes a phase transition at 250K. The low-temperature structure (cubic  $\text{Pa}\bar{3}$ ) shows a twofold orientational disorder; the corresponding populations are in thermal equilibrium (Bürgi, H.-B. et al., *Angew. Chem. Int. Ed.*, 1992, 31, 640-643). We now report the high-temperature structure (cubic  $\text{Fm}\bar{3}\text{m}$ ) determined from published synchrotron X-ray data (Chow, P. C. et al., *Phys. Rev. Lett.* 1992, 69, 2943-2946). The room-temperature scattering density distribution has been parametrized in terms of a combination of oriented symmetry-related molecules, and of a freely spinning molecule. Corresponding populations are 61% and 39%. The oriented part of the model is obtained, in good approximation, by imposing symmetry  $\text{m}\bar{3}\text{m}$  on the energetically more favourable major orientation in the low-temperature structure of  $\text{C}_{60}$ . The orientational probability density distribution has been calculated from the molecular libration tensors. It shows maxima for  $\text{C}_{60}$  orientations possessing  $\bar{3}\text{m}$  crystallographic site symmetry. It is also relatively large for the  $\text{C}_{60}$  orientations with cubic site symmetry  $\text{m}\bar{3}$ . The smallest energy barrier for reorientation between different  $\bar{3}\text{m}$  orientations *via* a  $\text{m}\bar{3}$  orientation appears to be less than 2  $\text{kJ mol}^{-1}$ . On average, 75% of the intermolecular contacts of the oriented molecules are longer than those observed in the low-temperature structure, the other