PS10.11.11 ORIENTATIONAL FLUCTUATIONS, DIFFUSE SCATTERING AND ORIENTATIONAL ORDER IN SOLID C_{60}.

K. H. Michel*, J. R. D. Copley†, *Department of Physics, Universiteit Antwerpen UIA, 2610, Antwerpen, Belgium, †National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

Starting from a microscopic model of interactions between C_{60} molecules on a fcc lattice, we formulate the orientational interaction potential in terms of symmetry adapted rotator functions. All irreducible representations of the cubic group up to the manifold 1 = 12 are taken into account. We introduce new symmetry adapted normal coordinates for orientational motion. Physical quantities such as the free energy are formulated in terms of these normal coordinates. We calculate the diffuse scattering law throughout the Brillouin zone. The theory describes in a very satisfactory way recent X-ray and neutron scattering experiments. We study the orientational order parameter taking into account all T_{2g} and T_{1g} representations up to the manifold 1 = 10. The temperature evolution of the order parameter is obtained within molecular field theory from the selfconsistent solution of a transcendental equation. The coupling of representations largely enhances the transition temperature and the first order character of the phase transition.

PS10.11.12 RARE-GAS INTERCALATED C_{60}.*

B. Morosin, Sandia Nat'l Lab., Albuquerque, NM 87185, G.H. Kwei, Lawrence Livermore Nat'l Lab., Livermore, CA 94550, J.D. Jorgensen and S. Short, Argonne Nat'l Lab., Argonne, IL 60439 and J.E. Schirber, Sandia Nat'l Lab.

The intercalation of the rare gases into interstices of C_{60} at 0-6 kbar pressures has been studied by neutron diffraction using a gas pressure cell at the Intense Pulsed Neutron Source (Special Environment Powder Diffractometer). He intercalates easily while Ar does not; for Ne, intercalation kinetics may be monitored using lattice parameter changes as a function of time following sudden changes in Ne pressure. Intercalation rates decrease with increasing Ne pressure, with time constants on the order of several hours. Upon pressure release, diffusion out of the C_{60} occurs at rates too fast to measure by this technique (i.e., a few minutes).

The fcc-sc (Fm3m to Pa3) orientational ordering transition occurs at a pressure which is highest for He, intermediate for Ne and smallest for Ar, the latter with a value in agreement with literature values for several nonpenetrating media.[1] For each intercalated compound in either the fcc or sc phases, these data yield the room-temperature compressibilities.[2] Rietveld refinement of the time of flight data for the more extensive room temperature Ne data sets show that only the octahedral interstices are occupied with Ne, that there is a pressure dependence on the octahedral site occupancy, and that the cubic lattice parameter increases linearly with the amount of intercalated Ne. The observed lattice parameter behavior is similar to the problem of packing of hard spheres with large size dissimilarity, previously addressed with molecular dynamics calculations.[3] We believe that this is the first observation of this effect in a realistic physical system.

1. W.I.F. David et al., Proc. Roy. Soc. Lond. A**442** 129 (1993); J. Phys. Condens. Matter **5** 7923 (1993); G.A. Samara et al., Phys. Rev. B**47** 4756(1993).
2. J.E. Schirber et al., Phys Rev B**51** 12014 (1995).
3. D.L. Ermak et al., J. Phys. Chem. **85** 3221 (1981).

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PS10.11.13 CRYSTAL STRUCTURE AND PHASE TRANSITION OF FULLERENE C_{76}

H. Nakao, Y. Fujii ISSP, Univ. of Tokyo, T. Watanuki, K. Ishii, T. Ino, H. Suematsu, Dept. of Phys., Univ. of Tokyo, H. Kawada, Y. Murakami, KEK-PF, K. Kikuchi, Y. Achiba, Y. Maniwa, Tokyo Met. Univ.

High-resolution synchrotron x-ray powder diffraction experiments of a fullerene C_{76} crystal has elucidated its structure and successive phase transitions. Two types of crystal lattices, fcc and hcp, coexist with different stacking sequences as conventionally denoted by ABAB(hcp) and ABCABC(fcc). Lattice constants at room temperature are obtained as a=15.42Å (fcc) and a=10.93Å, c=17.72Å (hcp). A precise measurement of them reveals the following phase transition sequence with respect to molecular rotation:

[fcc]	Phase I (T<140K)	orientationally disordered glass state.
	Phase II (140K<T)	free rotation state.
[hcp]	Phase I (T<140K)	c/a = 1.60, orientationally ordered.
	Phase II (140<T<420K)	c/a continuously varied.
	Phase III(420K<T)	c/a=1.63, free rotation state.

Calculations of intensity by an ellipsoid-shaped molecular model suggest that in Phase I of hcp the long rotational axis of molecules aligns in the stacking direction. In Phase II a molecule starts rotation about its long axis whose direction fluctuates. By applying pressure we have also studied phase boundary between I and II of the hcp structure. The present experimental results qualitatively agree to the recent NMR studies[1]. We also discuss the lattice stability conditions by combining our previous works on C_{82}[2].

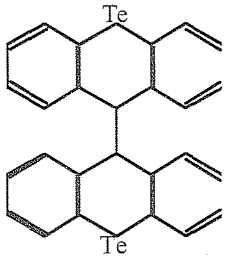
[1] Y. Maniwa et al., to be published.

[2] H. Kawada et al., Phys. Rev. B51,8723 (1995).

PS10.11.14 CRYSTAL STRUCTURES AND LUMINESCENCE PROPERTIES OF THE MOLECULAR COMPLEXES C_{60} AND C_{70} WITH 9,9'-trans-bis (TELLURAXANTENYL).

B.Zh.Narymbetov, S.S.Khasanov, L.P.Rozenberg, R.P.Shibaeva, E.A.Steinman, V.V.Kveder, D.V.Konarev+, R.N.Lyubovskaya+, Institute of Solid State Physics RAS, 142432 Chernogolovka, MD, Russia, +Institute of Chemical Physics RAS, 142432 Chernogolovka, MD, Russia.

The structures of molecular complexes C_{60} and C_{70} with 9,9'-*trans*-*bis*(telluraxantenyl) were determined by X-Ray analysis.



$\underline{C_{60}C_{26}H_{18}Te_2CS_2}$: a=10.309(1), b=10.988(3), c=12.011(1) è, α=85.20(2), β=71.85(1), γ=79.83(2)°, V=1271.9 Å^3, Sp.gr. P-1, Z=1; R=0.057 for 3983 refls. (MoK_α).
$\underline{C_{70}C_{26}H_{18}Te_2CS_2}$: a=10.927(3), b=21.068(5), c=24.147(7) è, V=5558.6 Å^3, Sp.gr. $Pbc2$, Z=4; R=0.101 for 1869 refls. (MoK_α).

Luminescence properties of these molecular complexes were investigated and compared with the corresponding properties of the initial C_{60} and C_{70}.

X-Ray experimental data for the single crystals of a molecular complex C_{60} with tetraphenyldipyranylidene were obtained: a=13.199(3), b=15.592(2), c=22.199(3) Å, α=102.87(1)°, V=4453.8 Å^3, Sp.gr. $I2$, Im or $I2/m$, 1806 refls. (MoK_α). It's crystal structure is in progress.