PS10.11.11 ORIENTATIONAL FLUCTUATIONS, DIFFUSE SCATTERING AND ORIENTATIONAL ORDER IN SOLID C_{60} 
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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 rotor functions. All irreducible representations of the cubic group up to the T_{1g} and T_{2g} representations to the manifold \( I = 10 \). The theory describes the orientational order parameter taking into account all T_{1g} and T_{2g} representations up to the manifold \( I = 10 \).

The temperature evolution of the orientational 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, Sandia Nat'l Lab., Livermore, CA 94550, J. D. Jorgensen and S. Short, Argonne Nat'l Lab., Argonne, IL 60439

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. For each intercalated compound in either the fcc or sc phases, these data yield the room—temperature compressibilities. 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. We believe that this is the first observation of this effect in a realistic physical system.

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PS10.11.13 CRYSTAL STRUCTURE AND PHASE TRANSITION OF FULLERENE C_{60} 

High-resolution synchrotron x—ray powder diffraction experiments of a fullerene C_{60} crystal have 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 \( a=15.42(1) \mathrm{AA}, c=17.72(1) \mathrm{AA} \).

Calculations of intensity by an ellipsoid—shaped molecular model suggest that in Phase I of hcp the long rotational axis of molecules aligns along the long axis whose direction fluctuates. 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 with the recent NMR studies. We also discuss the lattice stability conditions by combining our previous works on C_{60}.


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

The structures of molecular complexes C_{60} and C_{70} with 9,9’-trans-bis(telluraxanteny) were determined by X—ray analysis.

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