SOLID C_{60}: A NOVEL MATRIX FOR SMALL MOLECULES

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Solid C_{60} is a promising matrix for the storage of guest species, both *inside* and *in between* the cages. It consists only of one type of atoms, and the high molecular symmetry results in well-defined and uniform intercalation sites. In solid C_{60} (fcc lattice) there are, beside the void inside the C_{60} molecule, two types of interstitial sites that are available for intercalants, one octahedral site (d=4.1 Å) and two tetrahedral sites (d=2.2 Å) per C_{60} molecule. A reasonable estimate of the 'van der Waals length' of a CO molecule is 4.4 Å, suggesting that the CO molecule snugly fits into the octahedral sites of the C_{60} lattice.
Via high temperature, high pressure synthesis, samples in which large quantities of CO are trapped in these octahedral sites can be made. Under ambient conditions, the CO remains in the sample for many weeks.
The ro-vibrational motion of the CO molecules in the C_{60} matrix is studied as a function of temperature by infrared and nuclear magnetic resonance spectroscopy. The observed spectra indicate a gradual transition from nearly free motion of CO at room temperature to hindered motion at low temperature, with only tunneling between symmetry equivalent orientations remaining. The observations are augmented by theory, and details on the local environment of the CO molecules are extracted.