Crystallographic Studies of Fullerene Supramolecular Structures

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Recent work in the crystallographic characterization of fullerenes and endohedral fullerenes will be reported. Our goals are the determination of the particular cage geometry of higher fullerenes and for endohedrals the location of the interior atoms relative to the cage carbon atoms. The utility of co-crystallization of fullerenes with other molecules, particularly porphyrins, will be discussed, and the influence of one constituents upon the other constituent will be discussed. For example, we find that co-crystallization of μ-O{Fe^{III}(OEP)}$_2$ (OEP is the dianion of octaethylporphyrin) with C_{60} promotes pronounced bending of the μ-O{Fe^{III}(OEP)}$_2$ molecule. For recent published results see: 1. Lee, H. M., Olmstead, M. M., Iezzi, E., Duchamp, J. C., Dorn, H. C., and Balch, A. L. Crystallographic Characterization and Structural Analysis of the First Organic Functionalization Product of the Endohedral Fullerene $Sc_3N@C_{80}$. J. Am. Chem. Soc., 2002, 124, 3494-3495. 2, Olmstead, M. M., de Bettencourt-Dias, A., Stevenson, S., Dorn, H. C., and Balch, A. L. Crystallographic Characterization of the Structure of the Endohedral Fullerene {$Er_2@C_{82}$ Isomer I} with C_s Cage Symmetry and Multiple Sites for Erbium along a Band of Ten Contiguous Hexagons. J. Am. Chem. Soc., 2002, 124, 4172-4173

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