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Use of Fluorinated Tetraphenylporphyrins for the Cocrystallization of Fullerenes. Marilyn Olmstead, Daniel Nurco, Dept. of Chemistry, Univ. of California, One Shields Ave. Davis, CA 95616 USA.

It is well-known that porphyrins and metalloporphyrins create cavities favorable to cocrystallization with C_{60} , C_{70} , and endohedral fullerenes, and they have played an important role in the crystal structure determinations of these spherical molecules. Stabilization of these structures has been attributed to van der Waals interaction of the curved surface of the fullerene with the cavity provided by the porphyrin plane and cupping of either ethyl or phenyl substituents. Weak charge-transfer interactions between the fullerene as an acceptor and the porphyrin as a donor have also been invoked. In this report we will describe three new structures involving fullerenes and fluorinated tetraphenylporphyrin ($H_2F_{20}TPP$). The electron-withdrawing effect of F on the donor porphyrin molecule evidently does not tip the balance away from a favorable architecture. Instead, the cocrystals are readily formed and provide a new crystal engineering tool for the crystallization of fullerenes. We will examine the role played by several weak intermolecular interactions, such as $C-F \cdots \pi$, $C-F \cdots F-C$, and symmetrical packing motifs in the stabilization of these structures. Part of the structure of $C_{60} \cdot 1.5H_2F_{20}TPP$ is shown above.

