Crystallographic Investigations of Endohedral Structures

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The results of recent structural studies from single crystal X-ray diffraction of several endohedral fullerenes will be presented. This will include cases where co-crystallization with a metalloporphyrin is needed to produce a suitable diffracting crystal (as described previously in Olmstead, M. M., de Bettencourt-Dias, A., Duchamp, J. C., Stevenson, S., Dorn, H. C., and Balch, A. L. Isolation and Crystallographic Characterization of $ErSc_2N@C_{80}$: an Endohedral Fullerene Which Crystallizes with Remarkable Internal Order. *J. Am. Chem. Soc*., **2000**, *122*, 12220-12226 and Olmstead, M. M., de Bettencourt-Dias, A., Duchamp, J. C., Stevenson, S., Marciu, D., Dorn, H. C., and Balch, A. L. Isolation and Structural Characterization of the Endohedral Fullerene $Sc_3N@C_{78}$. *Angew. Chemie Int. Ed.*, **2001**, *40*, 1223-1225) and cases where the endohedral crystallizes in an ordered form due to chemical modification. Structural data on two isomers of $Er_2@C_{82}$ reveal considerable disorder in the metal atom positions but reveal the cage geometries. The data on an adduct of $Sc_3N@C_{80}$ show that adduct formation occurs at a 5:6 ring junction rather than at a 6:6 ring junction and that the Sc_3N unit does not interact with the site of addition but produces small bulges on the fullerene surface.