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Surprising New Results Concerning the Endohedral Fullerene Structures of C_{80}, C_{82}, C_{84}, C_{86}, and C_{88}.
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Endohedral fullerenes—large, even numbered carbon cages with positively charged species inside—differ in many respects from their empty cage congeners. All known empty cage fullerenes obey the isolated pentagon rule (IPR) in which pentagons are only fused to hexagons. We have already reported the first single crystal structure determination of a non-IPR endohedral fullerene, $Sc_3N@C_{68}$, where three pentagon-pentagon fusions occur in a D_3 symmetric arrangement. Moreover, among the seven possible IPR isomers of C_{80}, the I_h isomer is predicted to be the least stable, but in the set of endohedral molecules $M_3N@C_{80}$ (M=Sc, Y, Lu, or lanthanide), the I_h isomer is the most stable. We now report a number of structures which feature some of the following surprises: a second isomer of $M_3N@C_{80}$ with D_{5h} symmetry; a second non-IPR endohedral fullerene, $Tb_3N@C_{84}$; an egg-shaped fullerene of $Tb_2(C_2)@C_{88}$ as well as a new isomers of M_3N clusters within C_{86} and C_{88}. Examination of these structures reveals clues about the formation of fullerenes, information about the distribution of charge within the fullerene cages and the strength of π-π intermolecular interactions between the fullerene and cocrystallized porphyrin molecules.