

W0427

**Tb<sub>3</sub>N@C<sub>84</sub>-- A Non-IPR isomer of C<sub>84</sub>.** Christine M. Beavers, Marilyn M. Olmstead, Alan L. Balch, Univ. of California, Davis & Harry C. Dorn, Virginia Polytechnic Institute and State Univ.

A new isomer of C<sub>84</sub> was recently determined from the structure of an endohedral metal nitride fullerene co-crystallized with nickel octaethylporphyrin (NiOEP). Tb<sub>3</sub>N@C<sub>84</sub> was isolated and characterized by mass spectrometry to have the stated formula, but the isomer was unknown. The surprising result was that the fullerene cage violated the Isolated Pentagon Rule (IPR), making it part of an exclusive group of known Non-IPR fullerene structures. Non-IPR fullerenes have fused five-membered rings. This 5,5 bond is relatively electron rich; the greater electron density is demonstrated by the totally ordered terbium atom  $\pi$ -bonded to the 5,5 junction. The other two terbium atoms in the nitride were disordered, with the major conformation appearing at approximately fifty percent occupancy. The fullerene cage itself has interesting structural aspects. It has two distinct ends: a pointed beak where the fused pentagons reside, and a rounded end that resembles half of a C<sub>80</sub>. These ends are joined by a contiguous band of ten hexagons. The beak end has mm symmetry, but the round end has fivefold rotational symmetry. Overall, the fullerene has m symmetry. This new isomer will be compared to more symmetric IPR endohedral fullerenes with respect to nitride orientation, and co-crystallization  $\pi$ -stacking.

