Toward the direct synthesis of higher fullerenes

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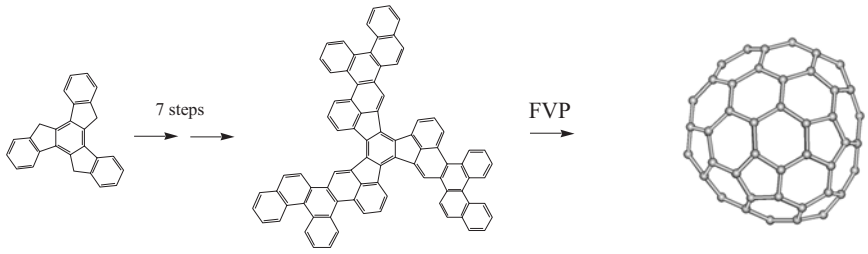
The main task of direct synthesis is the controlled generation of the desired fullerene cages by rational chemical synthesis. This approach is of practical interest as method of synthesis of individual higher fullerenes, including isomers which cannot be obtained during the uncontrolled process of graphite vaporization. Despite the great success in the total synthesis of many complex organic molecules, the rational construction of fullerene cages still remains challenging for organic chemistry, mostly because of their non-planar π-system resulting in very high strain energies.

Starting from truxene C_{60}, C_{78}(4) and C_{84}(20) fullerene related structures containing all carbon atoms in appropriate positions for fullerene cage formation have been synthesized and have been investigated as pyrolytic precursors for direct fullerene synthesis. Isolable quantities of C_{60} fullerene have been achieved by intramolecular condensation of a precursor containing all 60 carbon atoms and 72 out of the 90 required C-C bonds [1]. The pyrolysis of a precursor containing all 78 carbon atoms in the required positions and 93 of the 117 C-C bonds, needed for fullerene formation, showed selectivity for C_{78} fullerene formation under flash vacuum pyrolysis conditions (FVP) [2]. The C_{84} precursor containing more than 83% of C_{84}-(20) fullerene connectivity (105 of the 126 C-C bonds) was synthesized through an 8 step synthesis and investigated as a pyrolytic precursor. The MS data confirm a highly selective formation of C_{84} fullerene under FVP conditions [3].



Taking into account that higher fullerenes are not being formed selectively by random assembling during pyrolysis, the formation of higher fullerenes from corresponding precursors provide the evidence of the direct fullerene formation by FVP. Through independent experiments, it has been shown that the FVP of fullerenes is not affected by Stone-Wales rearrangement, which makes the FVP technique very promising for the synthesis of individual isomers of higher fullerenes.

[1] K.Yu. Amsharov, and M. Jansen, J. Chem. Sciences 62b, 1497 (2007).
[2] K.Yu. Amsharov, and M. Jansen, J. Org. Chem.73, 2931 (2008).
[3] K.Yu. Amsharov, and M. Jansen, Chem. Comm. accepted (2009).