Higher Fullerene Precursors, Toward the Direct Synthesis of Higher Fullerenes.

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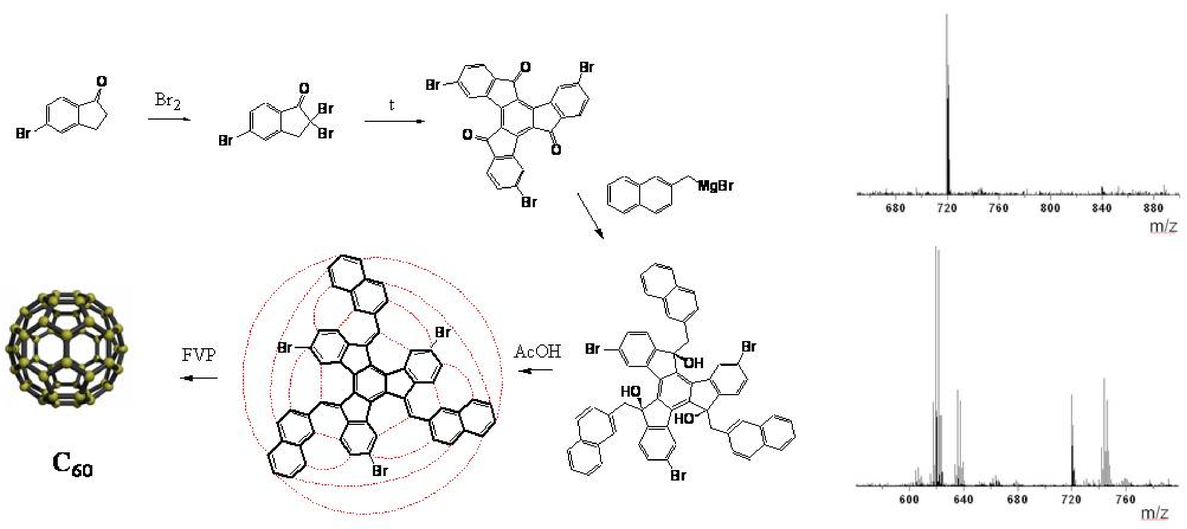
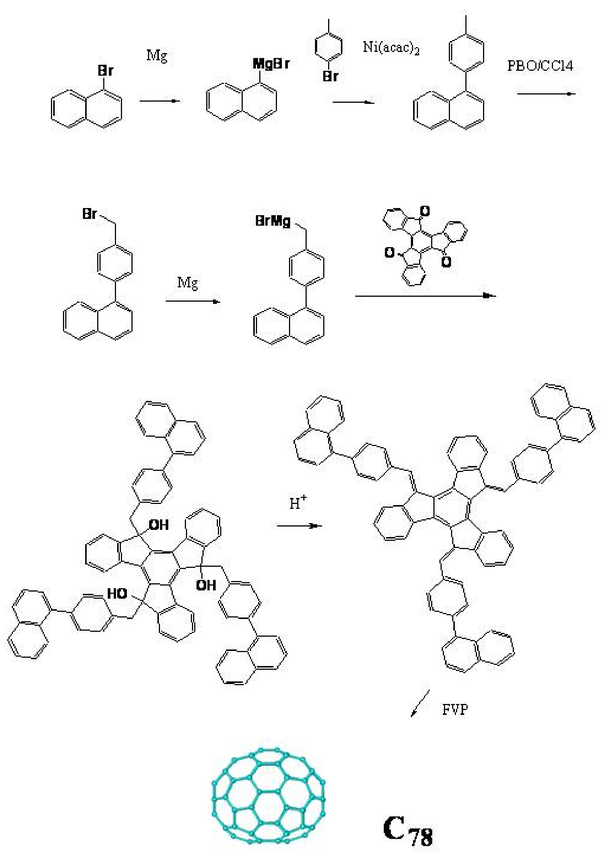
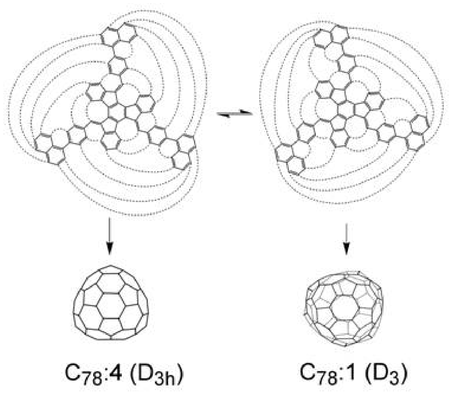
Direct synthesis of fullerenes is of practical interest as a prospective method for obtaining new fullerene species which can not be synthesized in the uncontrolled process of graphite evaporation, as well as for higher fullerenes which are formed in low yields as hard-to-isolate mixtures. Starting from truxene (truxenone) C_{60}, C_{78}(4) and C_{84}(20) fullerene-related structures have been synthesized and have been investigated as pyrolytic precursors for direct fullerene synthesis.

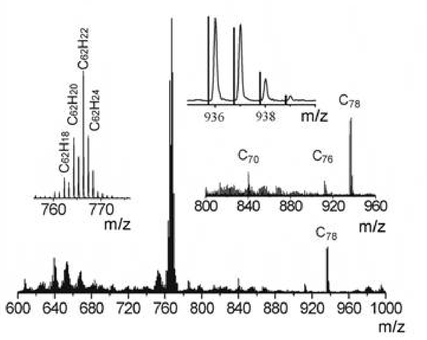


The truxenone molecule is a promising starting agent for the synthesis of halogenated precursors suitable for the generation of buckybowl and closed carbon structures through pyrolysis. Separable amounts of C_{60} were obtained through intramolecular condensation of a precursor containing all 60 carbon atoms in the appropriate positions, 72 of 90 required C-C bonds and 3 bromine atoms [1]. The relatively high and selective conversion makes such an approach very promising, especially concerning higher fullerenes which form in very small amounts or can not be obtained by the uncontrolled graphite evaporation technique.

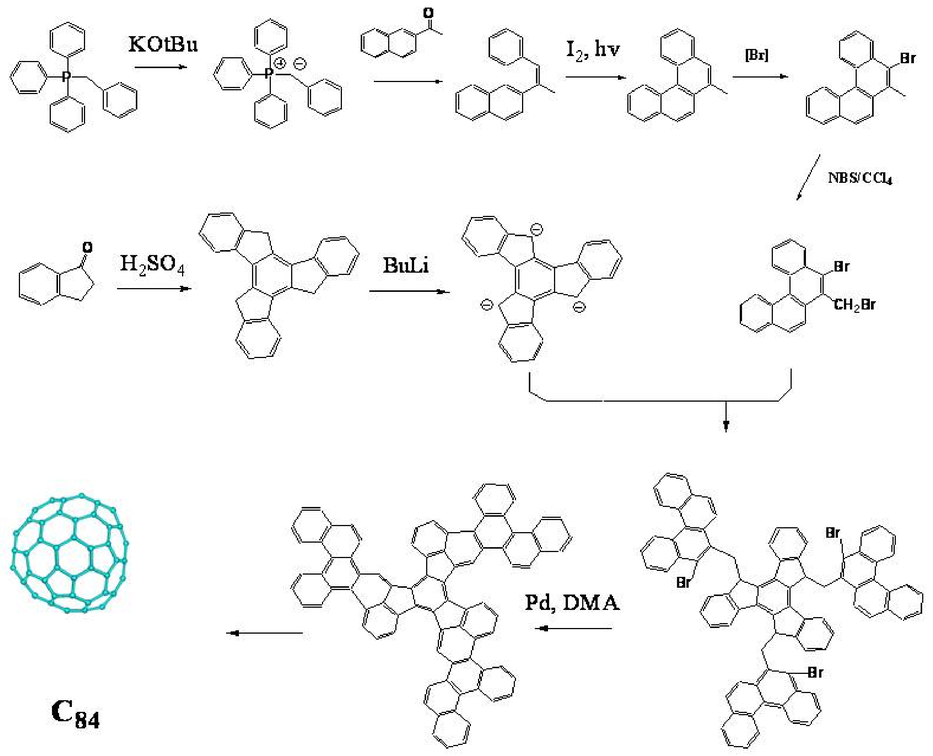


The C_{78}-fullerene related structure was obtained through a 6-step synthesis and investigated as a pyrolytical precursor. The pyrolysis of precursor containing all 78 carbon atoms in the required positions and 93 of the 117 C-C bonds needed for fullerene formation, showed selectivity for C_{78} fullerene formation according to MS data. Despite the relatively intense signals in the mass spectra the attempts to isolate it by HPLC were unsuccessful. We believe that the low fullerene yield is probably a consequence of the presence of weak bonds in the initial precursor, which are not stable enough under FVP conditions. Taking into account that C_{78} fullerene is not being formed by random assembling during pyrolysis of different aromatic compounds unlike C_{60} fullerene, the results obtained are evidential of the direct fullerene formation by FVP [2].





The C_{84}-fullerene related structure was synthesized through a 9-step route. The precursor obtained contains all 84 carbon atoms in the required positions and does not contain any weak bonds. Presented molecule possesses more than 80% of C-C connectivity needed for C_{84} fullerene formation. The first FVP experiments have shown rather high thermal stability of the precursor. Remarkable intermolecular condensation with fullerene formation (MS data) were achieved only at very high temperatures about 1300°C. At the same time the partial decomposition and nonselective formation of C_{60} was detected at given conditions. We are optimistic that optimization of the precursor structure by introducing radical promoters will allow the pyrolysis temperature to be reduced and increase the selectivity of fullerene formation.



[1] K. Amsharov, M. Jansen // *Z. Naturforsch.* **2007**, (62b), 1497-1508
[2] K. Amsharov, M. Jansen // *J. Org. Chem.* **2008**. (73) , 2931-2934