Synthesis of 18π-Annulenic Fluorofullerenes (Trannulenes): A new generation of donor-acceptor materials.

Glenn A. Burley,[a] Anthony G. Avent,[a] Olga V. Boltalina,[b] Ilya V. Goldt't,[b] Dirk Guldi,[c] Massimo Marcaccio,[d] Francesco Paolucci,[d] Demis Paolucci[d] and Roger Taylor[a]

[a] *School of Chemistry, Physics and Environmental Sciences, University of Sussex, Brighton, UK BN1 9QJ.*
[b] *Chemistry Department, Moscow State University, Moscow, 119899*
[c] *Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556, U.S.A.*
[d] *Dipartimento di Chimica "G. Ciamician", Università degli Studi di Bologna, 40126 Bologna, Italy*

In the continual quest for candidates that necessitate efficient and long-lived electron/energy transfer processes, [60]fullerene derivatives have shown to be candidates worthy of study. However, one major drawback of using [60]fullerene derivatives as electron acceptor units is their reduced electron affinity resulting from saturation of one or more carbon-carbon double bonds. Fluorination of the fullerene sphere however *enhances* electron affinity (3.1 eV for $C_{60}F_{18}$[1] cf. 2.67 eV for C_{60}[2]), rendering fluorofullerenes as potentially superior electron-accepting moieties.

Of the fluorofullerenes available, trannulenes (Figure) provide:

1. A simple preparative route (one-step synthesis via triple nucleophilic substitution of tertiary carbanions with $C_{60}F_{18}$).
2. Stability in a range of solvents.
3. Attractive physicochemical properties [extensive visible absorptions (ε_{608} = 13,265; ε_{667} = 20,580), enhanced electron accepting ability ($E_{0/1}$ – 0.54 V cf. -1.06 V for C_{60})].

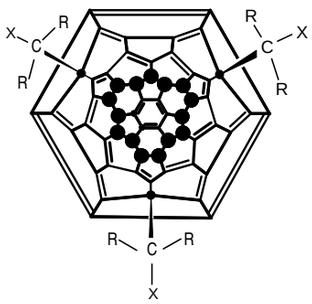

Figure: General structure (Schlegel) diagram of [18]trannulenes. (R = CO_2Et, X = electron withdrawing group, • = F).

This presentation will describe the factors that control trannulene formation and the preparation of multi-component donor-acceptor ensembles comprising the trannulene nucleus.

References

1. K. Ohkubo, R. Taylor, O. V. Boltalina, S. Ogo, and S. Fukuzumi, *Chem. Commun.*, 2002, 1952.
2. C. Brink; L.H. Anderson; P. Hvelplund; D. Mathur; J. Volstad *Chem. Phys. Lett.* 1995, 233, 52.