Electric field catalyzed Diels-Alder reaction of C_{70} with cyclohexa-1,3-diene

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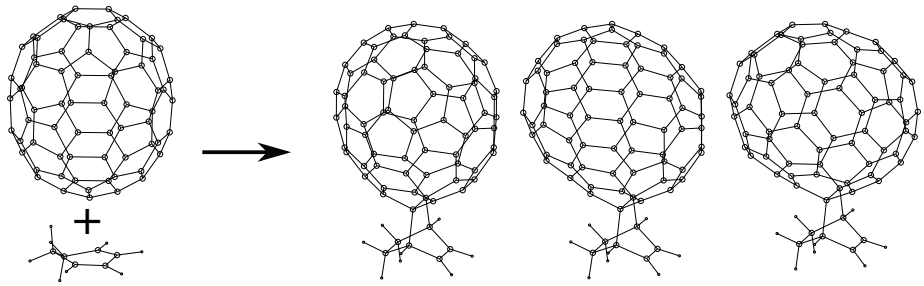

Reaction 1: *Diels-Alder reaction of C_{70} with cyclohexa-1,3-diene with list of reasonable regioisomers of product. Double bonds are not marked.*

C_{70} is a fullerene with prolonged ellipsoidal shape and D_{5h} symmetry. The structure consist of eight distinct groups of C-C bonds. Three of them have enough double bond character, so that they may react in Diels-Alder reaction. Reaction with cyclohexa-1,3-diene serves as the simplest meaningful model of anchoring C_{70} onto graphite sheet.

The influence of uniform external electric field (EEF) on the energetics of reaction 1 is studied by DFT methods on B97D3/Def2SVP level of theory. Reaction kinetics are analyzed through master equation implemented in Multiwell software[1].

The EEF affects the reactions towards three products differently, which may be used for improving stereoselectivity.

References

[1] J. R. Barker, T. L. Nguyen, J. F. Stanton, C. Aieta, M. Ceotto, F. Gabas, T. J. D. Kumar, C. G. L. Li, L. L. Lohr, A. Maranzana, N. F. Ortiz, J. M. Preses, J. M. Simmie, J. A. Sonk, P. J. Stimac, MultiWell-2017 Software Suite, `http://clasp-research.engin.umich.edu/multiwell/`, **2017**.