Molecular Modeling of Fullerene-Porphyrin Dyads

Peter Jarowski,[1] Stephen Wilson[1] and David Schuster[1]

[1]New York University
Department of Chemistry
100 Washington Square East
New York, NY 10003
USA

Computational studies were performed on C60-porphyrin dyads with varying linkers. Calculations were carried out using the Unix based computer programs Insight II and Spartan SGI. Using the Discover and Discover II modules in Insight II, both minimization and dynamics were performed under the forcefields ESFF and CFF91. Spartan SGI was used to calculate properties such as dipole moment, HOMO-LUMO energy gap, volume, and surface area. The study was done in order to assess the potential electron- transfer state properties of these systems with respect to molecular topology, i.e., donor-acceptor intramolecular distances. Surprising results were obtained in certain cases where these distances were calculated to be much smaller than would be predicted from traditional pictorial representations. Conformational as well as stereochemical properties greatly affected the resulting minimum energy topologies. The work lead to further empirical investigation of systems of interest in order to validate the computational findings. These new experimental results will be presented.

Support by the National Science Foundation is gratefully acknowledged.