

Molecular Dynamics and Energy Transfer Rates for Bifunctional Non-Conjugated Dendrimers.

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Abstract

In this research we present the results of structural studies using classical molecular dynamics (MD) simulations of bifunctional, non-conjugated, benzothiadiazole-based dendrimers with 3,5-dihydroxybenzyl alcohol as the repeat unit. Upon excitation the energy transfer occurs from the diarylaminopyrene donor units in the periphery to the benzothiadiazole-based chromophore, which acts as both the core and the acceptor. From the MD simulations we can obtain an ensemble of stable conformations and calculate energy transfer rate constants as a function of the generation of the dendrimer. This research was motivated by experimental results obtained for such dendrimers by the Thayumanavan group.* The experimental results suggest that the energy transfer rate constants scale with R^{-3} , where R is the distance between the donor and the acceptor. In contrast, Förster theory predicts that the rate constants should be proportional to R^{-6} . The simulations are designed to investigate the influence of dynamical effects such as backfolding on the magnitude and scaling of the energy transfer rate constants.

* K. R. J. Thomas, A. L. Thompson, A. V. Sivakumar, C. J. Bardeen, and S. Thayumanavan. "Energy and Electron Transfer in Bifunctional Non-Conjugated Dendrimers." *J. Am. Chem. Soc.* **2005**, *127*, 373-383.