

Abstract Submitted  
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**Conformational control in the photochemistry of hexatriene derivatives** DAN KIM, ENRICO TAPAVICZA, TRAVIS THOMPSON, California State University, Long Beach — The photochemistry of hexatriene (HT) is determined by the ground state equilibrium of different rotamers. Different side chains and their relative positions on the HT backbone structure have different effects on the equilibrium between the different rotamers. To investigate the influence of the side chains on the relative statistical weight of the rotamers at equilibrium, we studied HT and two of its derivatives: (3Z)-2-isopropyl-5-methylhexa-1,3,5-triene (IPMHT) and (3Z,5E)-3,7-dimethylocta-1,3,5-triene (DOT). To effectively sample the ground state equilibrium of these molecules we use ab initio replica exchange molecular dynamics (REMD) based on density functional theory (DFT). We perform the simulation with and without empirical correction for dispersion forces. Based on the equilibrium of structures in the ground state we calculate electronic absorption spectra using time-dependent DFT (TDDFT). Results from the study show that there is an influence of the conformation of the molecules on the excitation energy. This principle can be used to selectively excite a group of rotamers. Our calculated data will be compared to experimental data in order to determine the accuracy of the empirical correction for dispersion forces and if rotamers can be selectively excited experimentally.

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