PHOTO-REACTIVITY OF A PUSH-PULL MEROCYANINE IN A STATIC ELECTRIC FIELDS: A THREE STATE MODEL OF ISOMERIZATION REACTIONS INVOLVING CONICAL INTERSECTIONS

S. ZILBERG, X. F. XU, A. KAHAN and Y. HAAS, *Institute of Chemistry and the Farkas Center for Light Induced Processes The Hebrew University of Jerusalem, Jerusalem, Israel*; ,.

The photochemistry of a prototype push-pull merocyanine is discussed using a simple three state model. As a derivative of butadiene, two isomerization reactions may take place, around the two double bonds of the butadiene backbone. As a molecule substituted by an electron donor and electron acceptor at opposite ends, its structure as well as its photochemistry are expected to be strongly affected by the environment. It is shown that varying the solvent polarity or the electric field, can lead to different photochemical products. In particular, the existence of conical intersections is found to depend on these external parameters. This work provides a theoretical foundation for ideas expressed by Squillacote et al.* concerning the electrostatic control of photochemical reactions.
*Squillacote, M.; Wang, J.; Chen, J. J. Am. Chem. Soc. 2004, 126, 1940.