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Transition and Excited States of 1,1'-azo-bis-1,2,3-triazole VLADIMIR GONCHAROV, Vanderbilt University, OLGA GONCHAROVA, Vertex Pharmaceuticals Inc., KALMAN VARGA, Vanderbilt University — A novel photochromic molecule has been recently synthesized[1]. The photo-isomerization of this nitrogen-rich small molecule is efficiently controlled by a xenon flash lamp suggesting a potential in photonic and molecular mechanics applications. We perform a synergistic quantum molecular dynamics (QMD), real-time time dependent density functional theory (TDDFT) and TDDFT- perturbation theory study to capture and elucidate the transition state, excitation energies and optical properties of the molecule. We also use it to test performance of recently developed real-time TDDFT method[2] to calculate hyperpolarizabilities and compare results with the Sternheimer method.

[1]Yu-Chuan Li et al. *J. Am. Chem. Soc.*, 2010, 132, 12172
[2]V. Goncharov, K. Varga, *Phys. Rev. B* 2010, submitted.

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