Excited-State Dynamics in Nitro-Naphthalene Derivatives: Intersystem Crossing to the Triplet Manifold in Hundreds of Femtoseconds

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Supporting Information

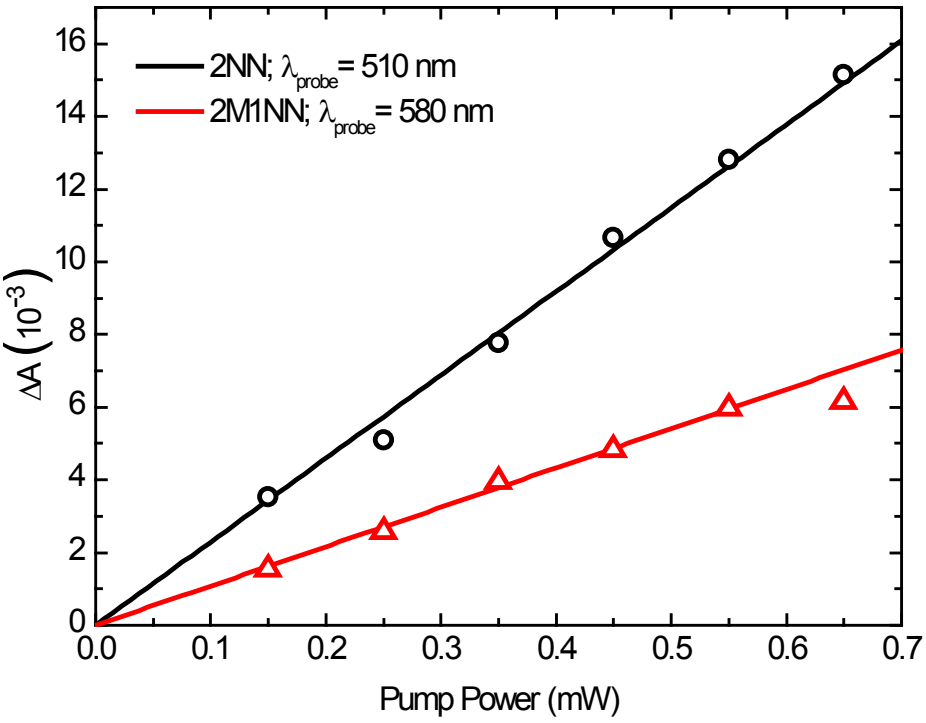

Figure 1S. Dependence of the triplet transient absorbance of 2NN and 2M1NN in acetonitrile solutions on the pump power. Measurements were taken at a delay time of 500 ps and at the probe wavelengths shown in the legend.

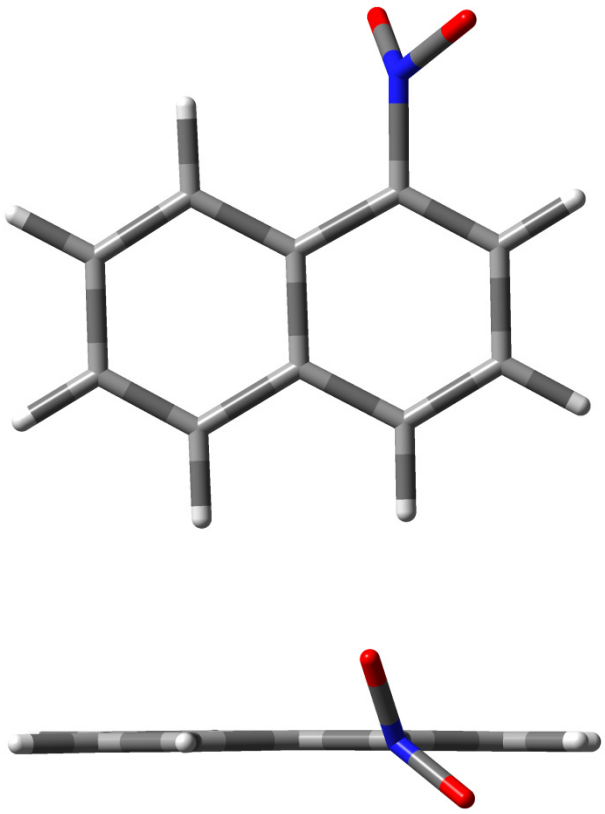

Figure 2S. Optimized S_1 state geometry of 1NN in acetonitrile at the CIS/IEFPCM/6-31+G(d,p) level of theory. Nitro-aromatic torsion angle, as defined in Fig. 1, equal to 75°. Note the pyramidal configuration of the nitro-group. The estimated transition energy and oscillator strength at this level of theory are 3.22 eV and 0.0083, respectively.