Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

The UVA response of enolic dibenzoylmethane: Beyond the static approach

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Supporting Information

Figure S1: Molar excitation coefficient of $\pi\pi^*$ (black line) and nπ^* (red line) states simulated by employing the classical (a) and quantum (b) computational protocols with 150 (full line), 100 (dashed line) and 50 (dotted line) points.

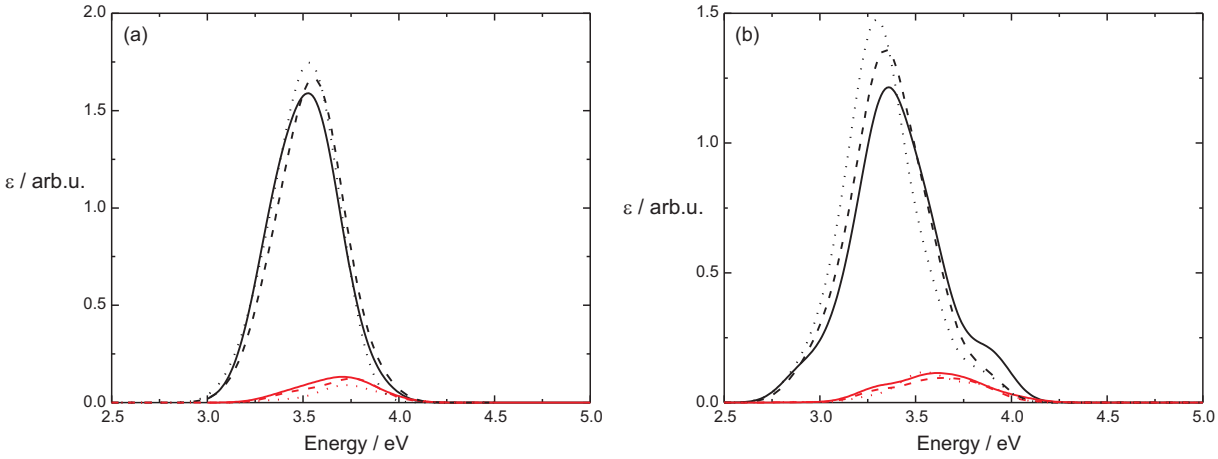

Figure S2: Correlation between the $\pi\pi^*$ excitation energies and the $\Delta(OH)$ coordinates sampled in the classical simulation. The Pearson correlation coefficient is 0.141.

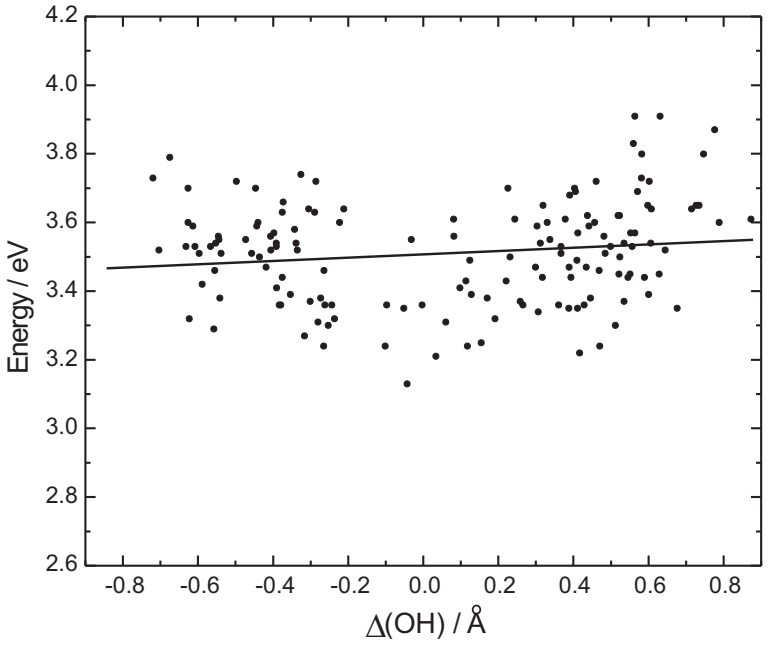

Figure S3: Correlation between the $\pi\pi^*$ excitation energies and the $d(CO)$ coordinate sampled in the classical simulation. The $d(CO)$ coordinate is a sum of two C-O bonds. The Pearson correlation coefficient is -0.274.

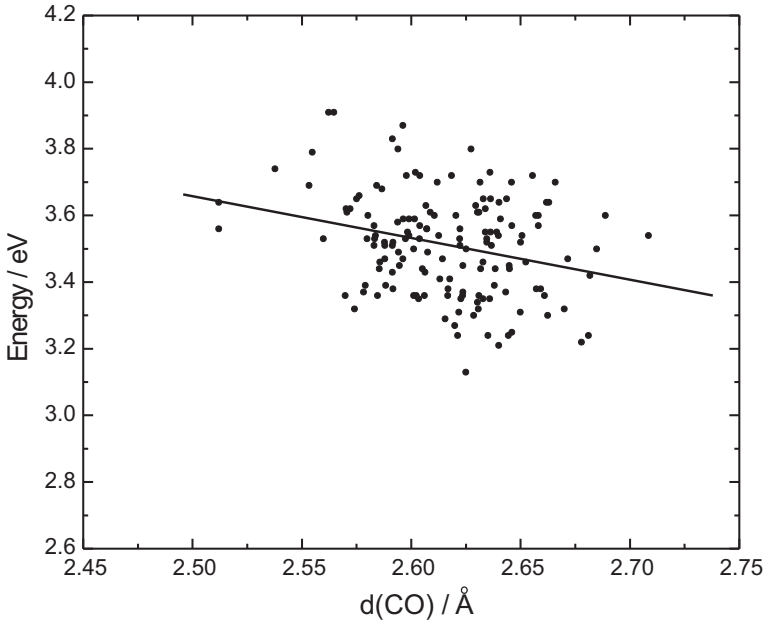

Figure S4: Correlation between the $\pi\pi^*$ excitation energies and the $d(C10 - C11)$ coordinates sampled in the classical simulation. The Pearson correlation coefficient is -0.068.

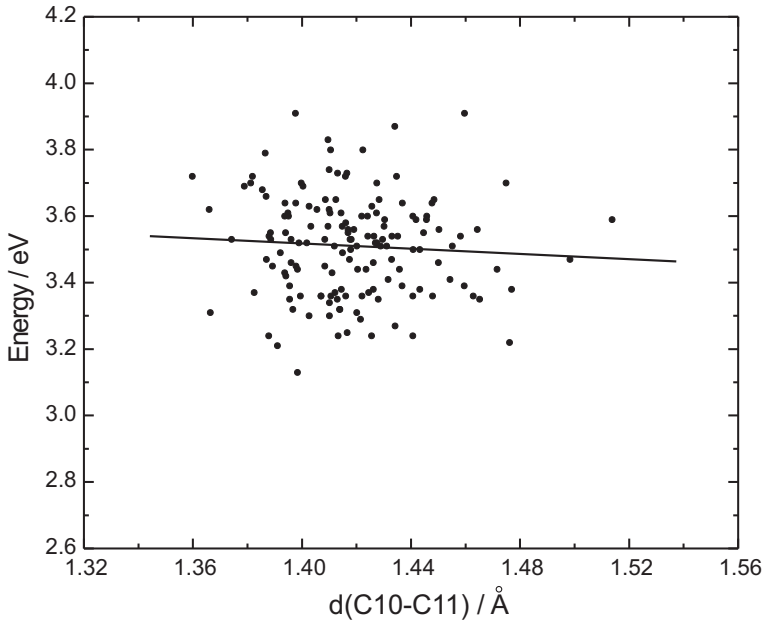

Figure S5: Correlation between the $\pi\pi^*$ excitation energies and the C1-C2-C3 angles sampled in the classical simulation. The Pearson correlation coefficient is -0.005.

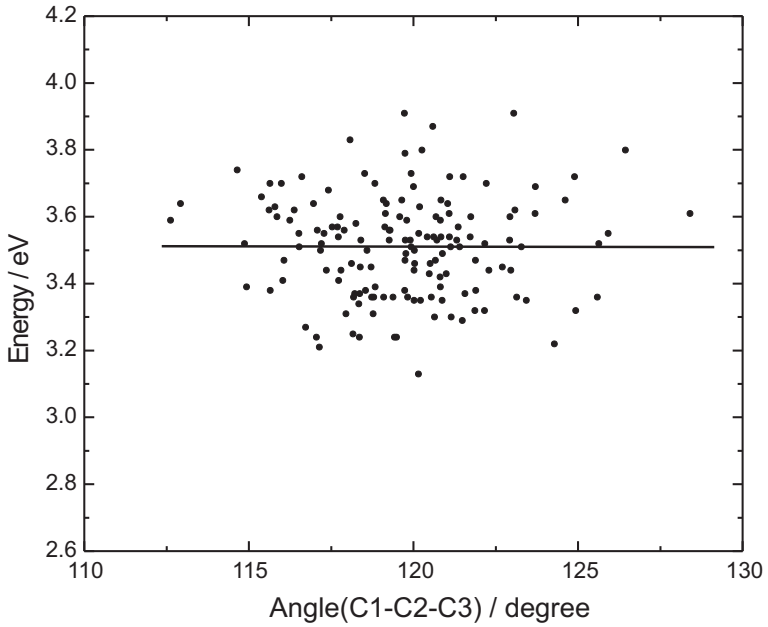

Figure S6: Correlation between the $\pi\pi^*$ excitation energies and the C11-C10-C1-C2 dihedral angles sampled in the classical simulation. The Pearson correlation coefficient is -0.033.

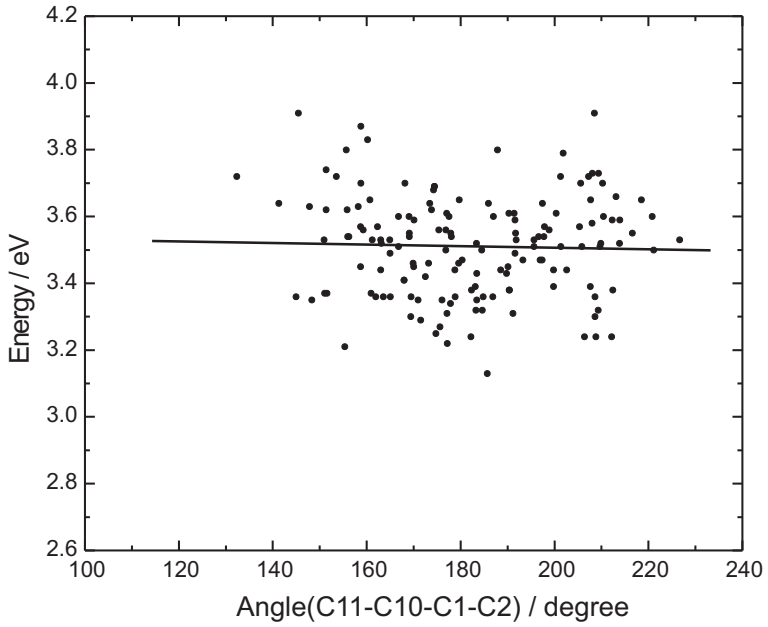

Figure S7: Correlation between the $\pi\pi^*$ excitation energies and the H-O1-C1-C2 dihedral angles sampled in the classical simulation. The Pearson correlation coefficient is -0.101.