Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

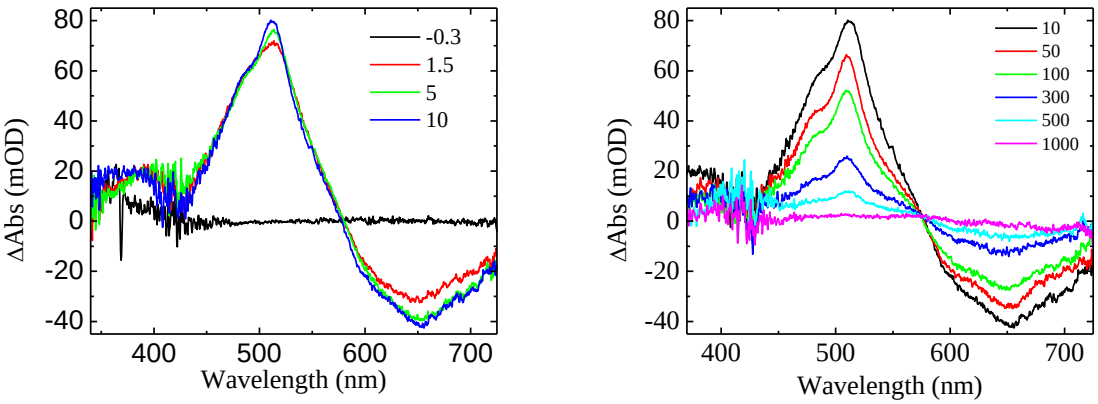

Fig S1. Transient Spectra at selected delays (ps) of isolated ***Ac***, λ_{exc}= 330 nm.

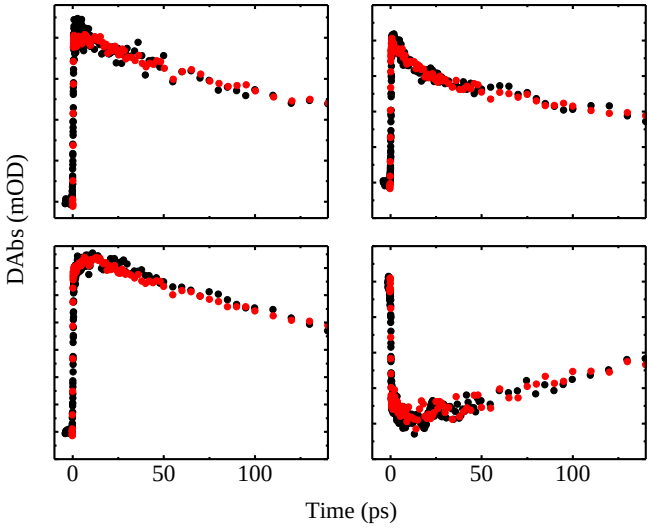

Fig S2. Kinetic traces of isolated ***Ac***, with λ_{exc}=330 nm *(black scatter)* and with λ_{exc}=400 nm *(red scatter)*.

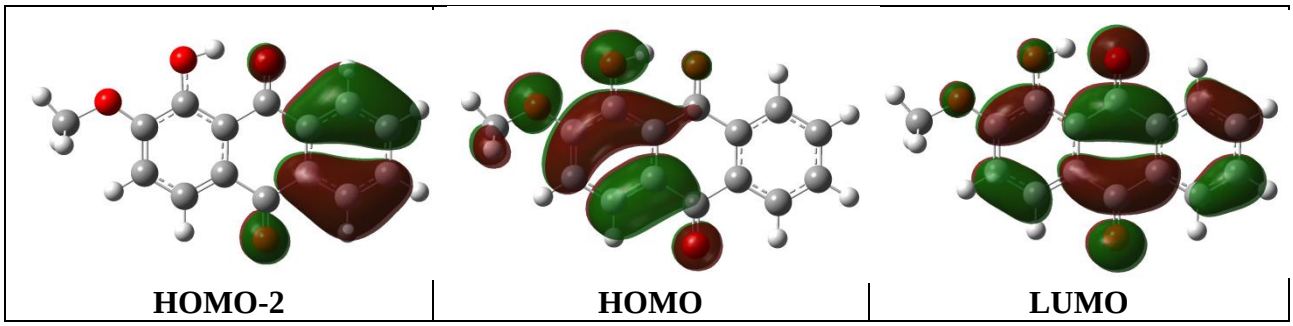

Fig S3: 3D plots of MO of interest of ***Ac***.

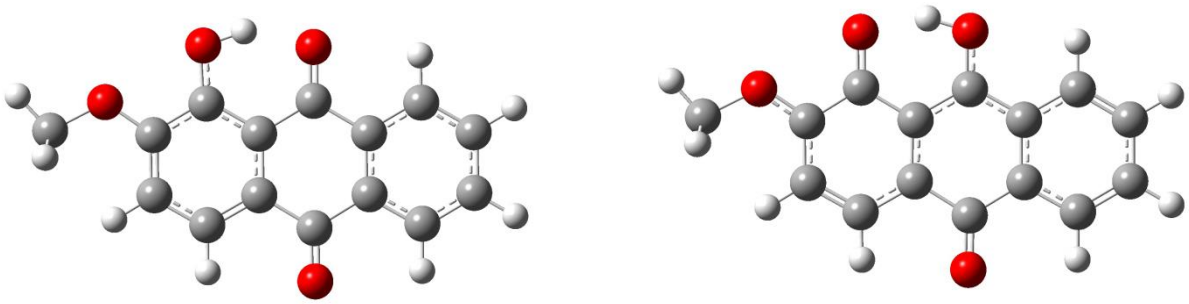

Fig S4: Ground electronic state (on the left) and first excited state (on the right) of ***Ac***.

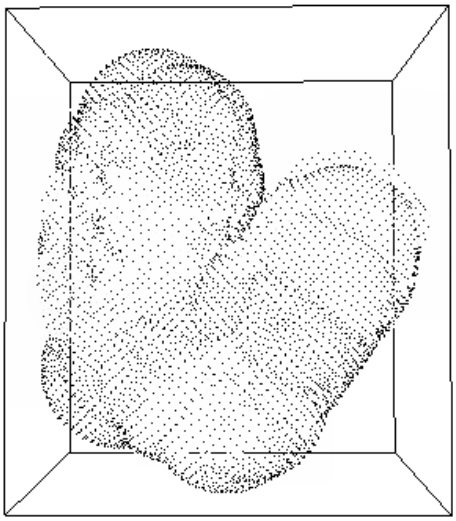

Figure S5: PCM cavity for the AAC conformation: solvent-accessible-surface (SAS).

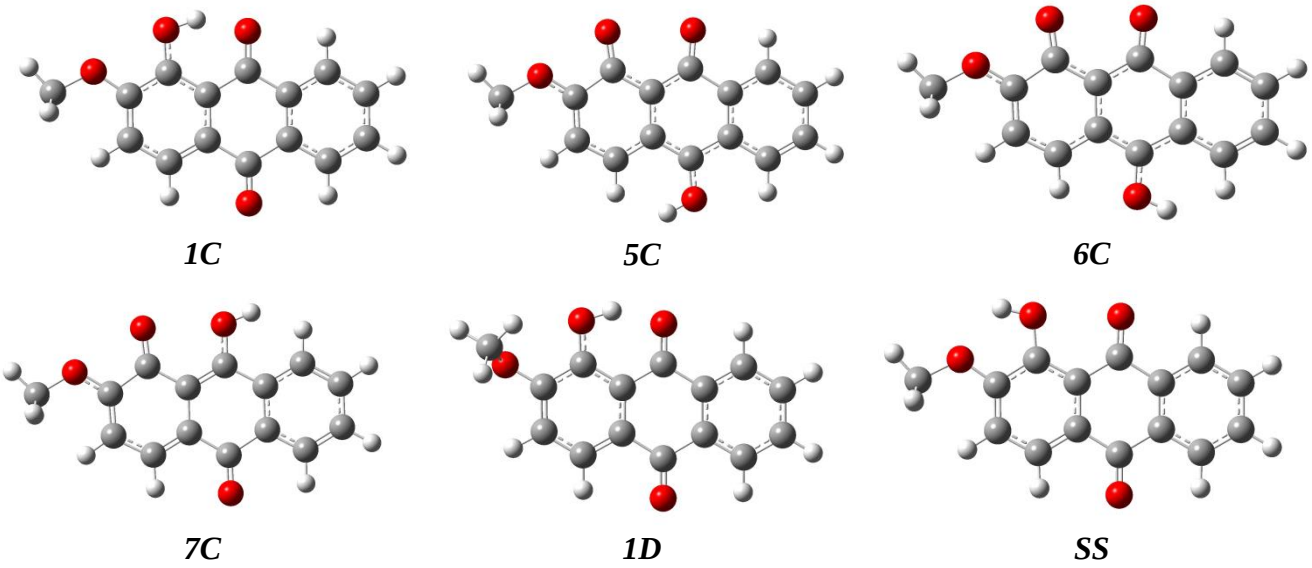

Figure S6. Relevant conformations of ***Ac***

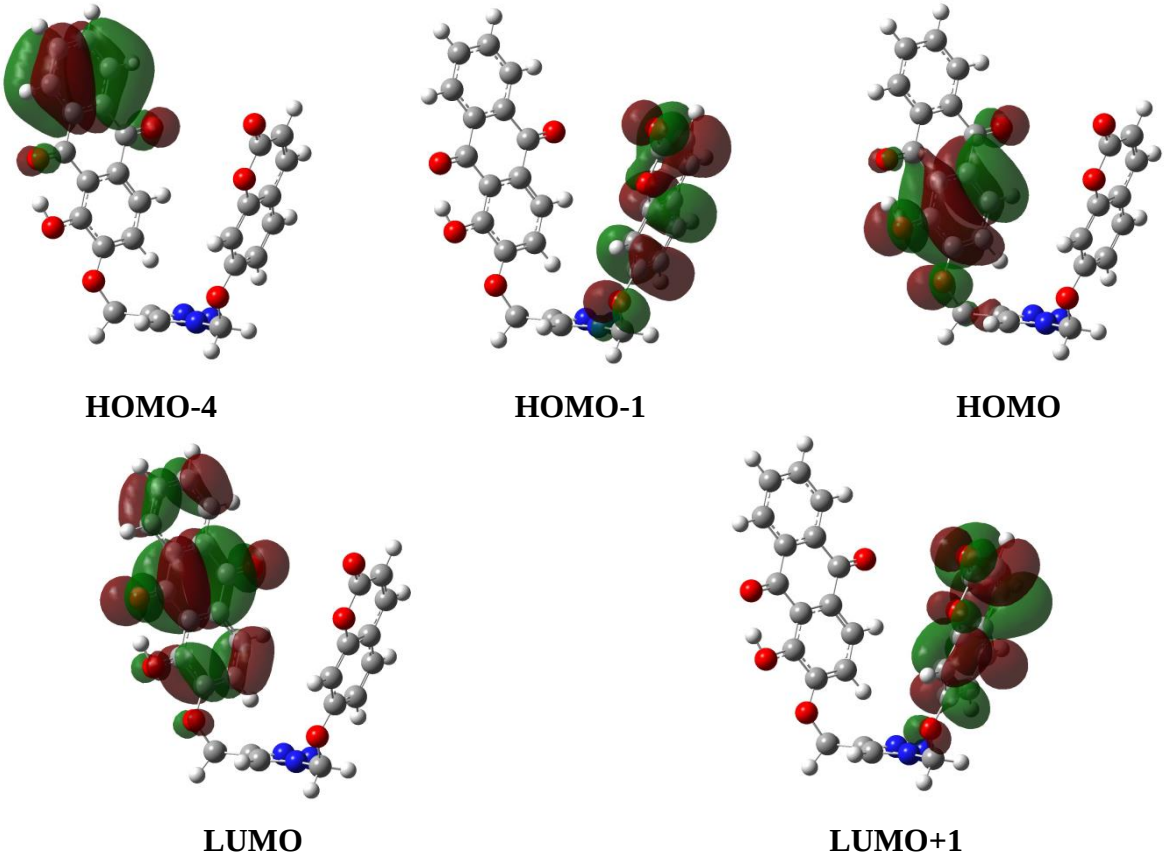

Figure S7: 3D plots of relevant MO of AAC.

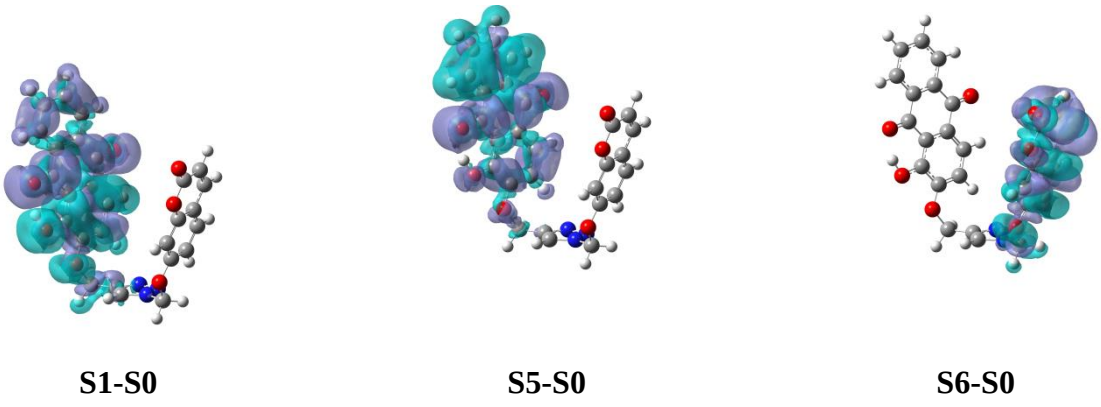

Figure S8: 3D plots of the electron density difference between the ground S0 and the first S1 (left-side picture), the fifth S5 (central picture) and sixth S6 (right-side picture) electronic state for AAC conformer. The zones where the electron density grows are mapped in light blue.

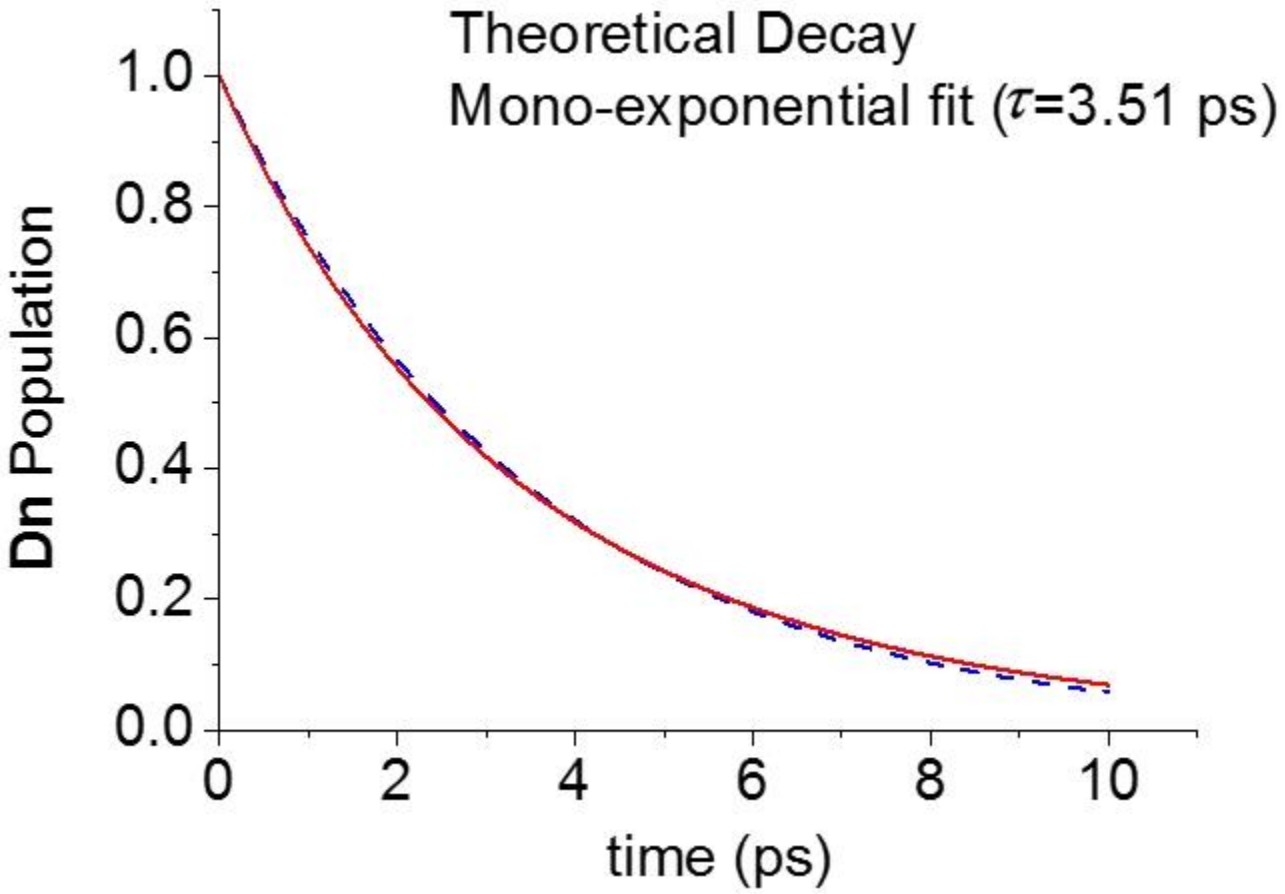

Figure S9: Theoretical ***Dn*** population decay due to the energy transfer, calculated assuming a weighted sum of exponential function (red line). The pre-exponential factors in the sum are the relative population of the conformers calculated by DFT approach. The dashed line is the mono-exponential fit, with a time constant of 3.51 ps.