

Supporting information

Monitoring the intramolecular charge transfer process in the Z907 solar cell sensitizer: A transient VIS and IR spectroscopy and ab-initio investigation

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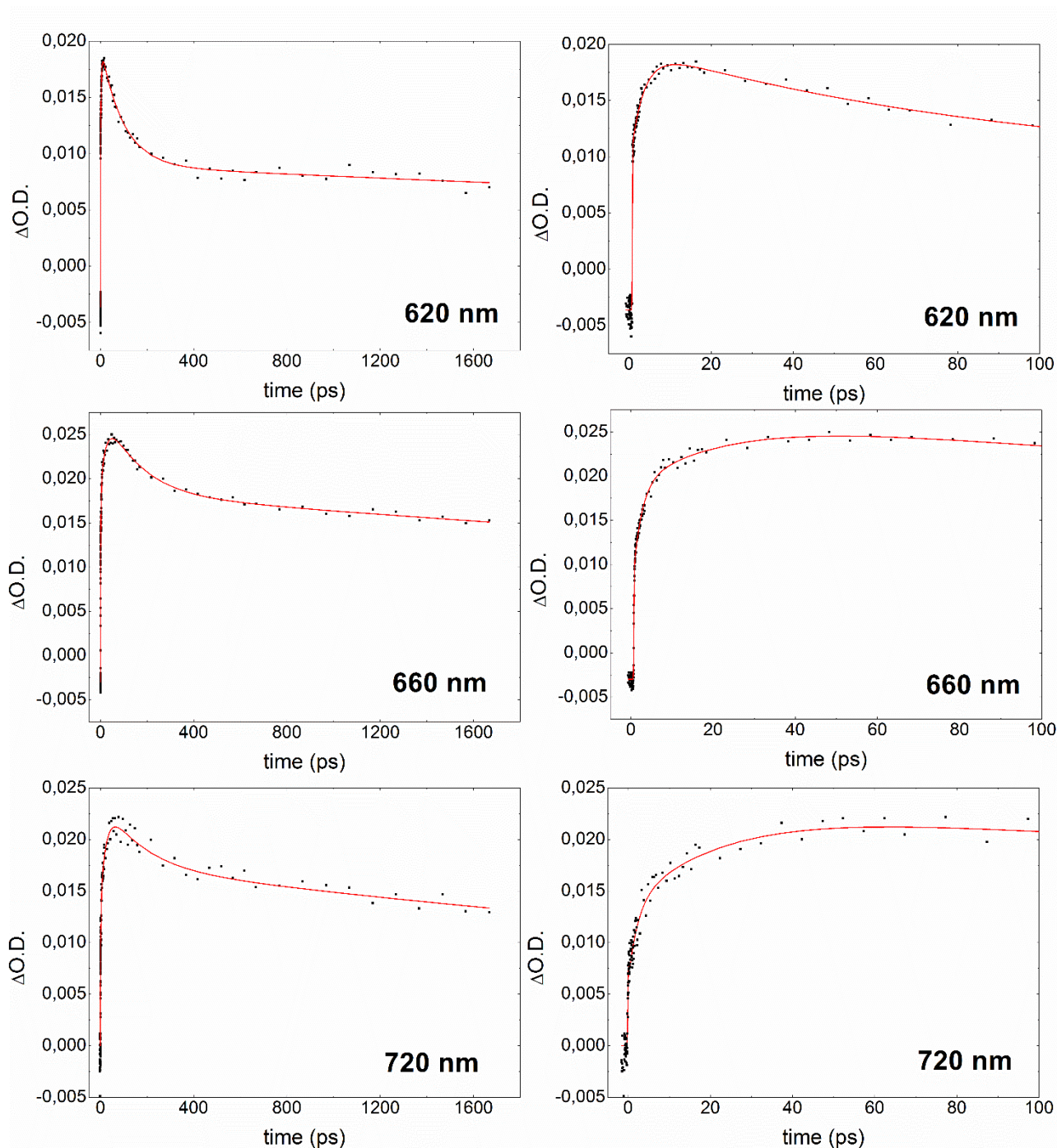


Figure S1 Experimental kinetic traces (black dots) and their fit (red lines) recorded at different wavelengths of Z907 in DMSO solution. On the left are reported the overall observed time interval. On the right only the first 100 ps are reported.

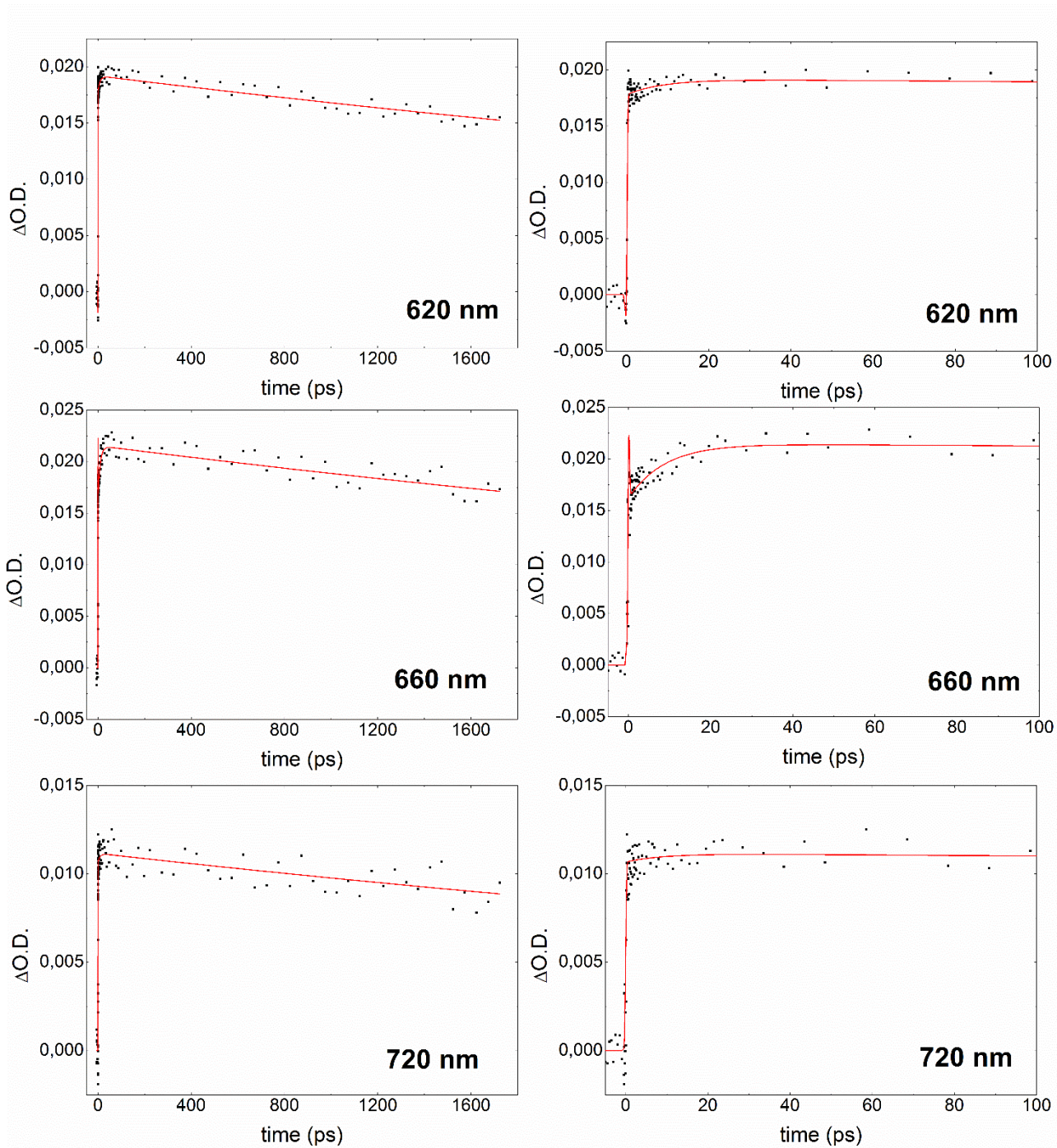


Figure S2 Experimental kinetic traces (black dots) and their fit (red lines) recorded at different wavelengths of Z907 in DMSO solution. On the left are reported the overall observed time interval. On the right only the first 100 ps are reported

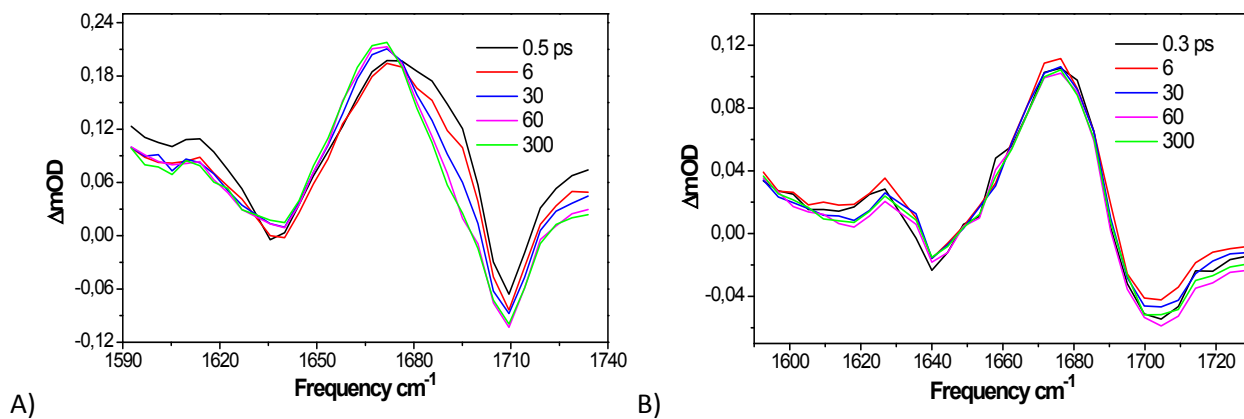


Figure S3: Selected time resolved spectra registered in the CO absorption region for Z907 dissolved in A) ETOH and B) DMSO.

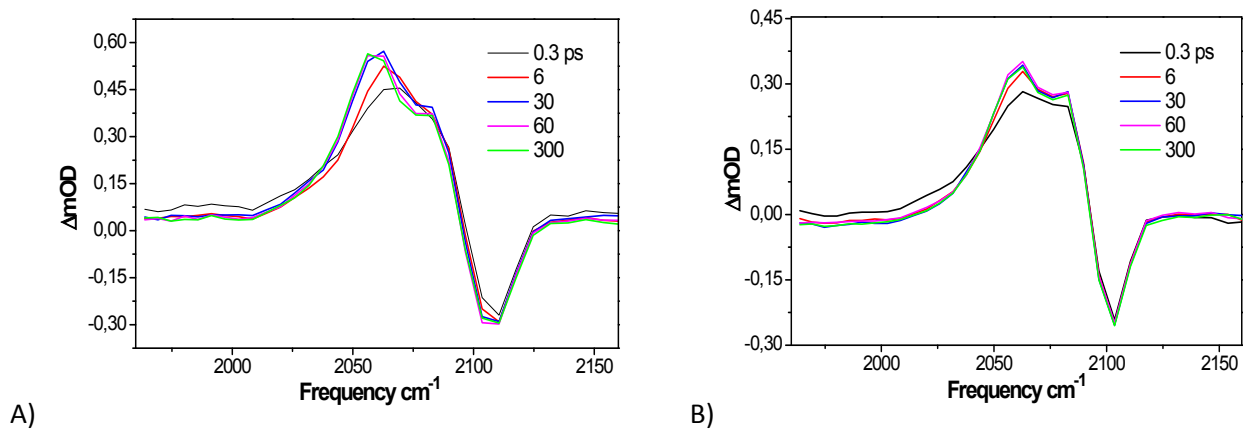


Figure S4: Selected time resolved spectra registered in the CN absorption region for Z907 dissolved in A) ETOH and B) DMSO.

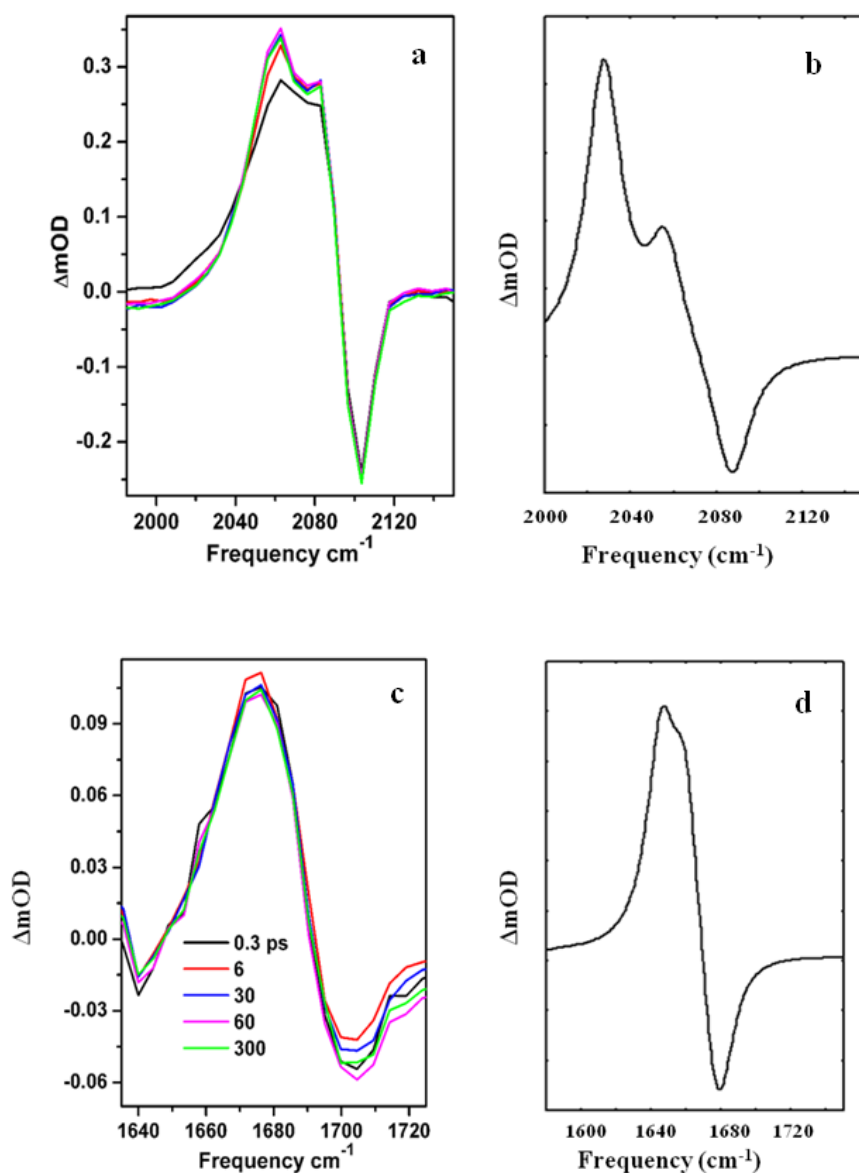


Figure S5: Transient infrared spectra of Z907 in DMSO excited at 520 nm and respective TDDFT simulation. a) experimental CN stretching region; b) simulated CN stretching region c) experimental CO stretching region; d) simulated CO stretching region.

The optical absorption spectra of the Z907, in both EtOH and DMSO, and of its hydrogen-bonded adducts, **Z907+2EtOH_NCS** and **Z907+2EtOH_COOH**, in EtOH are shown in Figure S6. While the position and intensity of the calculated $^1\text{LML}'\text{CT}$ band is basically unchanged going from EtOH to DMSO, a sizable red shift (ca. 0.2 eV) is predicted when the interaction with the solvent molecules moves from the thiocyanate ligands to the COOH groups, as a consequence of the increased charge accepting capability of the latter groups, resulting in an larger stabilization of the $^1\text{LML}'\text{CT}$ state. The interaction with the solvent again rationalizes the experimentally observed red-shift in EtOH, occurring on a 20-30 ps timescale, shown in the transient absorption spectra reported in Figure 3 in the article.

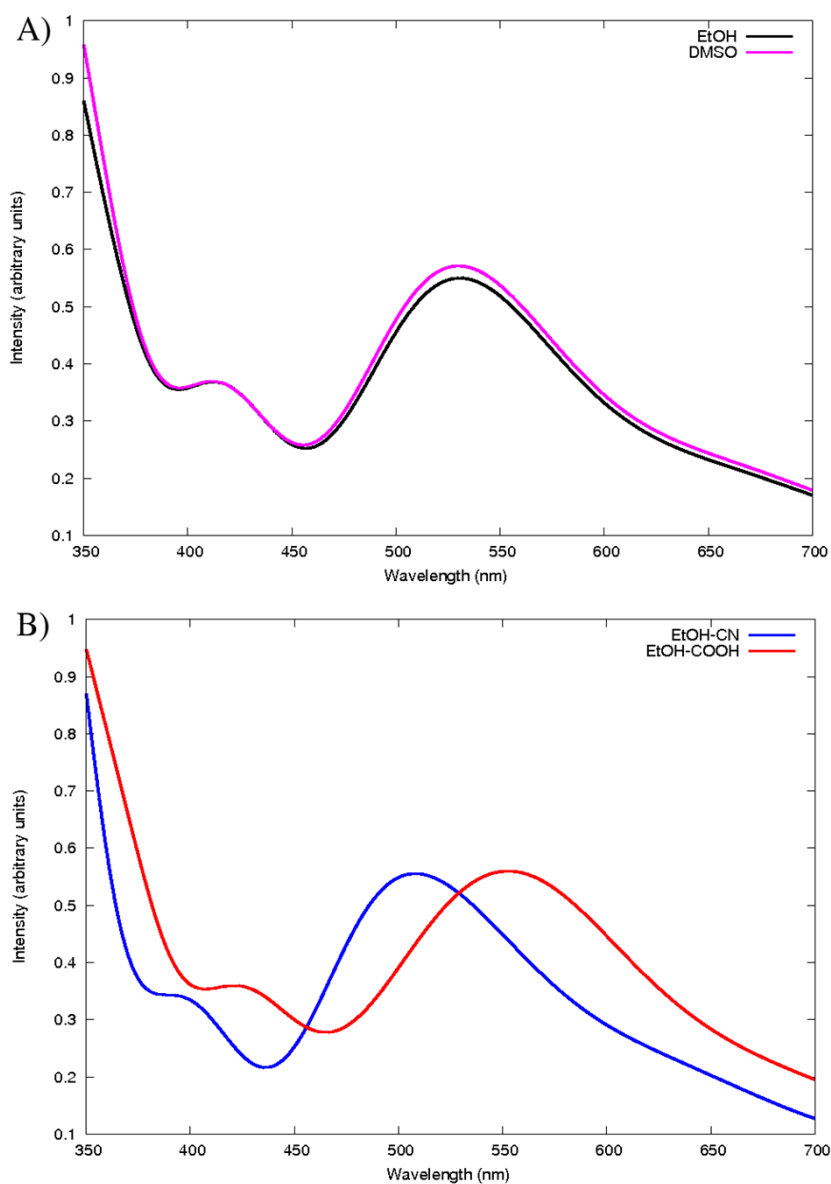


Figure S6. Calculated UV-Vis absorption spectra for **A)** Z907 in EtOH (black line) and DMSO (magenta line) and **B)** **Z907+2EtOH_NCS** (blue line) and **Z907+2EtOH_COOH** (red line) in EtOH. The calculated spectra were shifted of 0.23 and 0.25 eV in EtOH and DMSO, respectively, to make the maxima of the lowest $^1\text{LML}'\text{CT}$ band coincident with the experimental maximum (2.34 eV).