Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


Electronic Supplementary Materials

# Time Evolution of Entanglement of Electrons and Nuclei and Partial Traces in Ultrafast Photochemistry

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Supplementary Figures

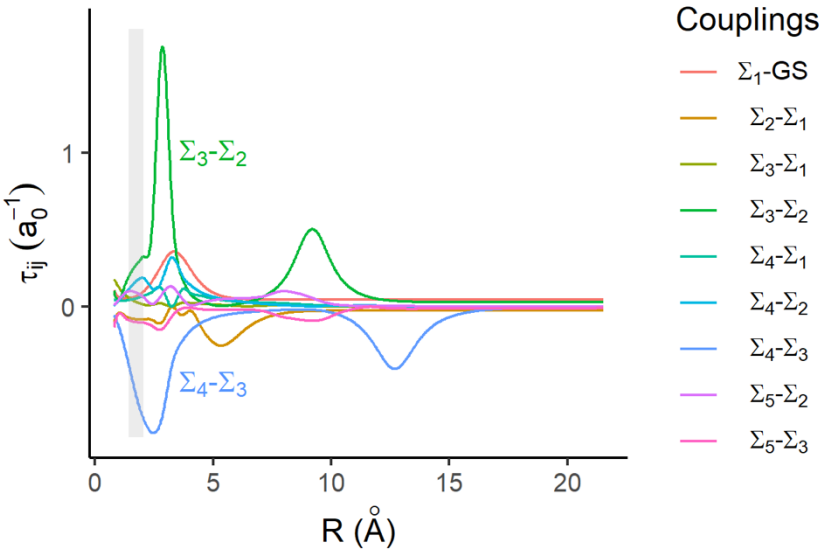


Figure S1 : Curves of the non adiabatic couplings, adapted from S. van den Wildenberg, B. Mignolet, R. D. Levine and F. Remacle, *J. Chem. Phys.*, 2019, **151**, 134310.

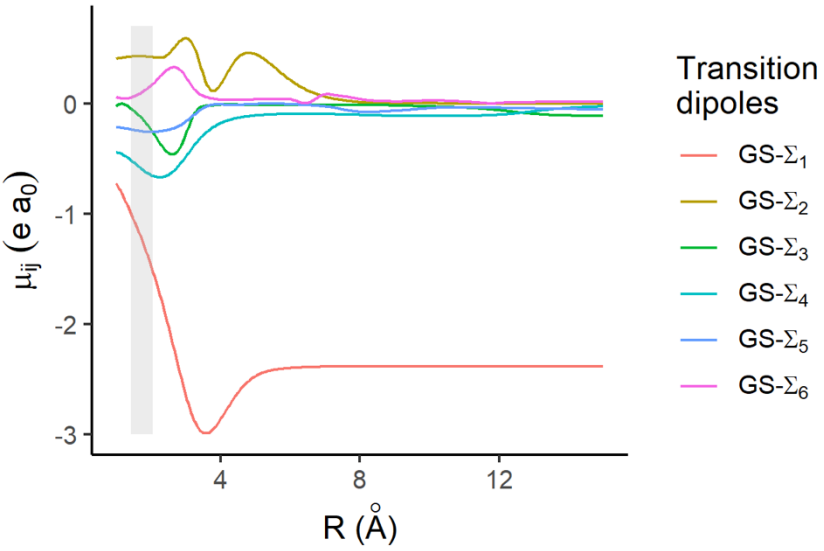


Figure S2 : Curves of the transition dipoles between the GS and the excited electronic states, adapted from S. van den Wildenberg, B. Mignolet, R. D. Levine and F. Remacle, *J. Chem. Phys.*, 2019, **151**, 134310.

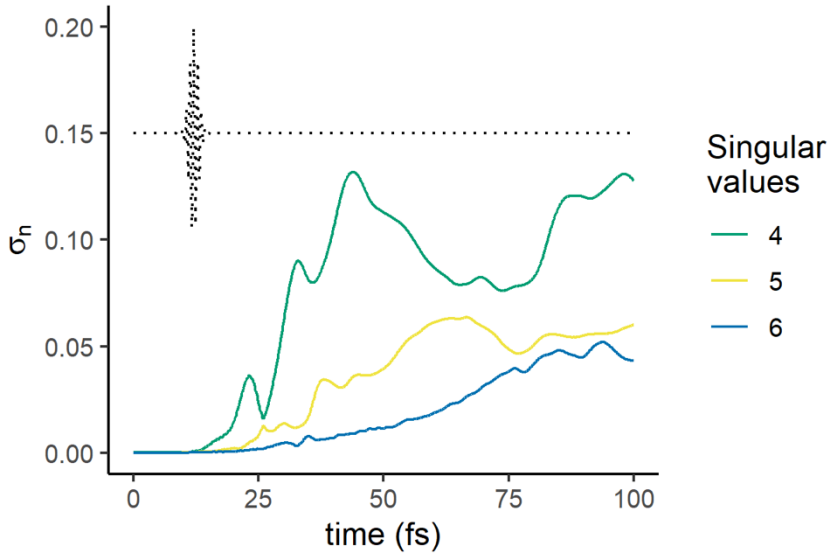


Figure S3. Zoom on the time dependence of the singular values $\sigma_4$, $\sigma_5$ and $\sigma_6$. The avoided crossings between $\sigma_4$ and $\sigma_5$ at 25 fs, and between $\sigma_5$ and $\sigma_6$ at 75 fs reflect the effect of the NAC coupling on the singular components. The weights of the electronic singular eigenvectors interchange in the regions of strong NAC.

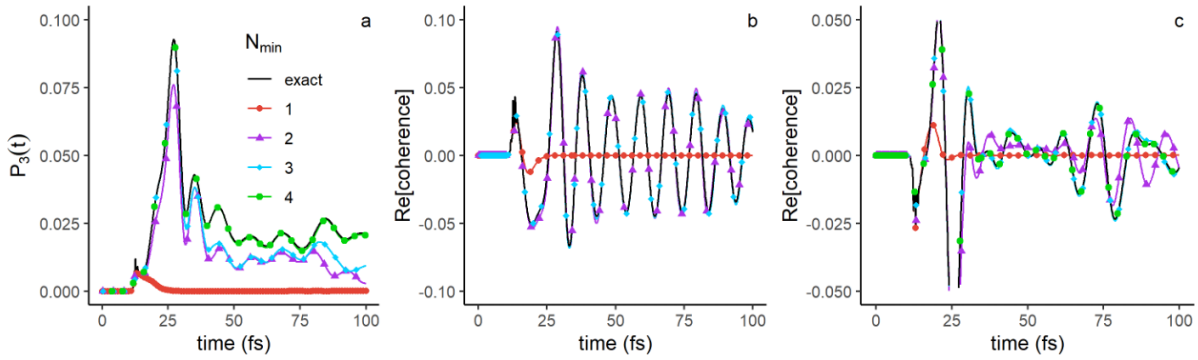


Figure S4. a) Recovered population of the $\Sigma_3$ state as a function of the number, $N_{min}$, of singular components included in Eq. (4). b) Recovered electronic coherence between the $\Sigma_3$ and the $\Sigma_4$ state. c) Recovered electronic coherence between $\Sigma_3$ and $\Sigma_2$. The color code is given in the inset of panel a.