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

Supporting information

Solvent reorganization triggers photo-induced solvated electron generation in solvated phenol

Isolde Sandler, Juan J. Nogueira,*‡ and Leticia González*

Institute of Theoretical Chemistry, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria.
‡ *Current Address: Research School of Biology, Australian National University, Acton, ACT 2601, Australia.*

Corresponding authors:

J.J.N. juanjose.nogueiraperez@anu.edu.au, L.G. leticia.gonzalez@univie.ac.at

Figure S1 Comparison between the absorption spectra calculated with ADC(2) and CC2 for phenol in the gas phase as well as for the 5 water molecules cluster model

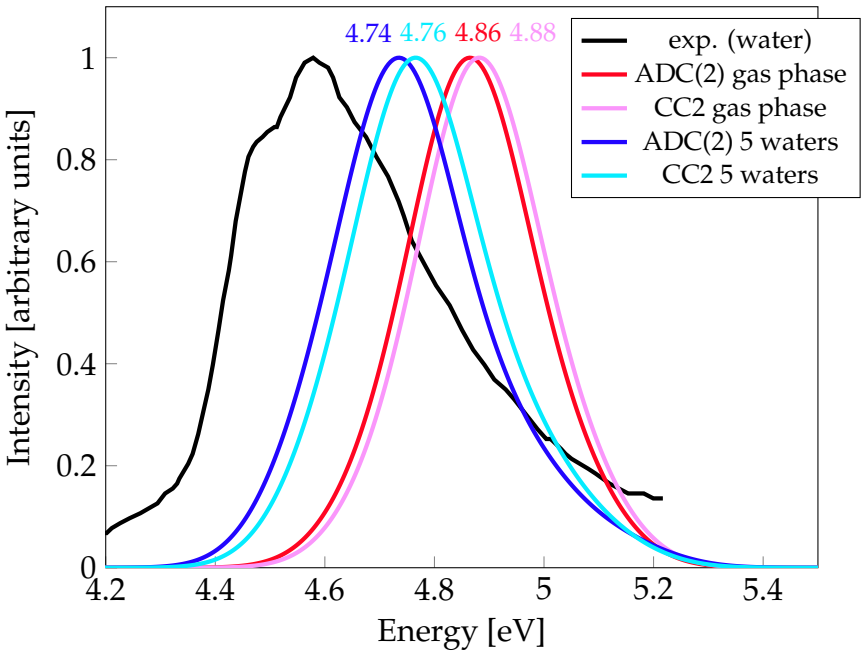

Figure S2 Comparison between the electronic structure analysis of absorption spectrum and density of states calculated with ADC(2) and CC2 for phenol with a cluster model comprised of 5 water molecules

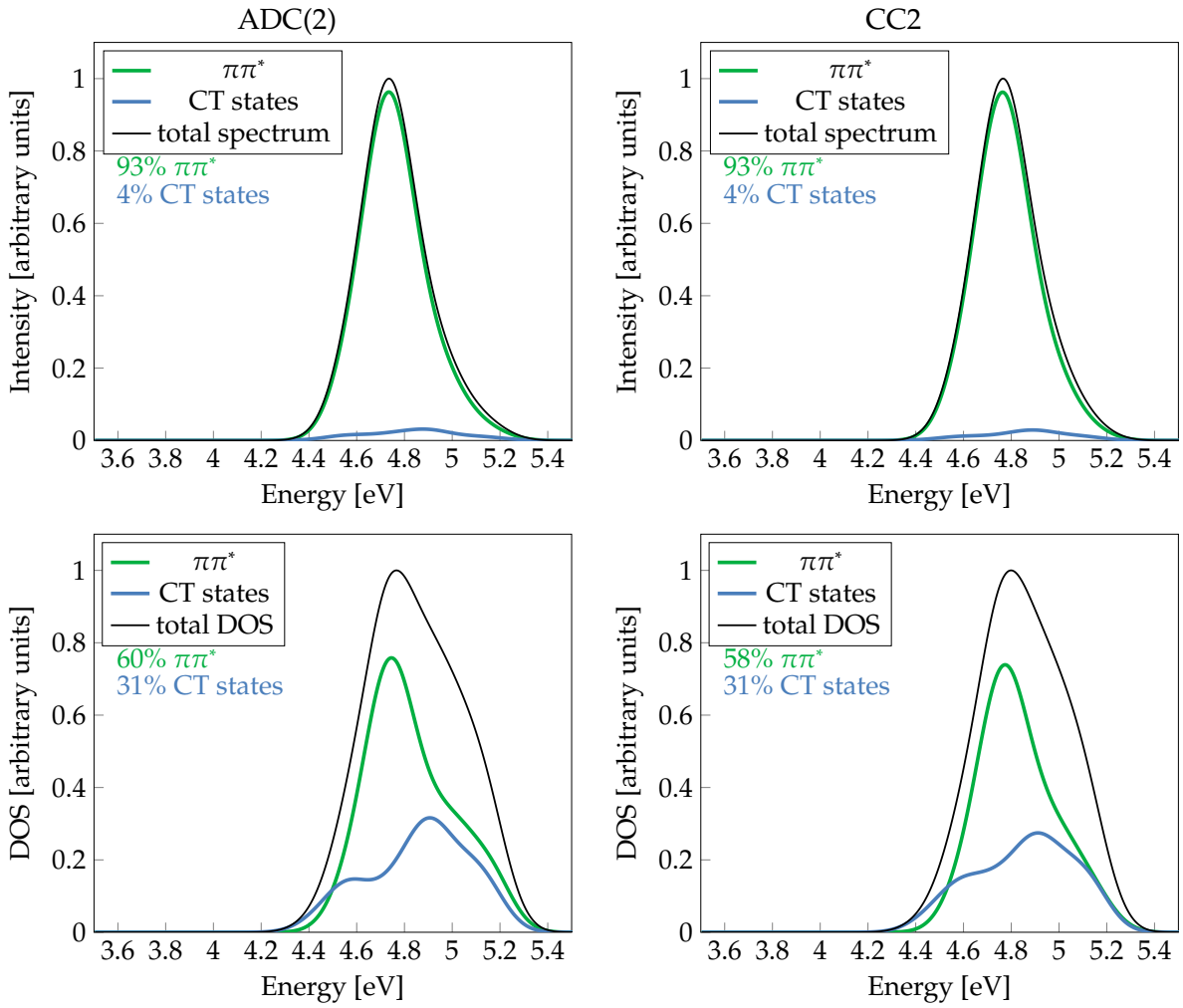

Table S1 Excitation energies [eV], oscillator strengths and state characters of a representative geometry with excitation energy close to the maximum of the $\pi\pi^*$ absorption band (highlighted in bold) for cluster models with different numbers of water molecules calculated with ADC(2). State characters are characterized by inspection of the natural transition orbitals.

	gas phase			1 water			5 waters			15 waters		
state	energy	osc.	char	energy	osc.	char.	energy	osc.	char.	energy	osc.	char.
1	4.91	0.027	$\pi\pi^*$	4.78	0.036	$\pi\pi^*$	4.81	0.033	$\pi\pi^*$	**4.80**	0.029	$\pi\pi^*$
2	5.45	0.001	Rydberg	5.00	0.001	CT	5.11	0.001	CT	5.58	0.002	CT+Rydberg
3	5.94	0.011	Rydberg	5.56	0.007	Rydberg	5.56	0.005	CT+Rydberg	5.83	0.079	$\pi\pi^*$+Rydberg
4	6.12	0.011	$\pi\pi^*$+Rydberg	5.78	0.004	Rydberg	5.76	0.011	CT	6.05	0.004	CT
5	6.27	0.018	Rydberg	5.88	0.058	$\pi\pi^*$	5.87	0.023	CT+Rydberg	6.25	0.002	Rydberg
6	6.33	0.008	Rydberg	6.04	0.023	$\pi\pi^*$+Rydberg	5.99	0.042	CT+$\pi\pi^*$	6.37	0.017	CT

Table S2 Excitation energies [eV], oscillator strengths, and state characters of a representative geometry with low charge-transfer state excitation energy (highlighted in bold) for cluster models with different numbers of water molecules calculated with ADC(2). State characters are characterized by inspection of the natural transition orbitals.

	gas phase			1 water			5 waters			15 waters		
state	energy	osc.	char.	energy	osc.	char.	energy	osc.	char.	energy	osc.	char.
1	4.92	0.053	$\pi\pi^*$	4.59	0.001	CT	4.58	0.000	CT	**4.49**	0.000	CT
2	5.04	0.001	Rydberg	4.79	0.058	$\pi\pi^*$	4.74	0.056	$\pi\pi^*$	4.86	0.052	$\pi\pi^*$
3	5.57	0.007	Rydberg	5.10	0.007	CT+Rydberg	4.94	0.010	CT+Rydberg	5.06	0.002	CT+Rydberg
4	5.86	0.065	$\pi\pi^*$+Rydberg	5.41	0.001	Rydberg	5.30	0.007	CT+Rydberg	5.53	0.008	CT
5	5.90	0.091	$\pi\pi^*$+Rydberg	5.50	0.065	$\pi\pi^*$+CT	5.38	0.022	CT+Rydberg	5.62	0.003	CT
6	6.32	0.014	Rydberg	5.75	0.014	Rydberg	5.51	0.016	CT+Rydberg	5.758	0.092	CT+$\pi\pi^*$