Electronic Supplementary Information (ESI) for: Photorelaxation of Imidazole and Adenine via Electron-Driven Proton Transfer Along H_2O Wires

Rafał Szabla,[*a] **Robert W. Góra,**[*b] **Mikołaj Janicki,**[b] **and Jiří Šponer**[a,c]

May 29, 2016

Table 1 Vertical excitation energies (in eV) of imidazole and adenine in the gas phase and their corresponding clusters with 5 water molecules, computed using the ADC(2)/aug-cc-pVDZ method assuming the ground-state minimum energy structures optimized at the B3LYP/def2-TZVP level. Since only the $\pi\sigma^*_{NH}$ states were relevant for the EDPT along H_2O wires mechanism the remaining excited electronic states of $\pi\sigma^*$ character were omitted in the main manuscript for clarity. These $\pi\sigma^*$ states had little effect on the overall excited-state dynamics of the isolated imidazole and its water cluster.

State / Transition		E_{exc}/[eV]	f_{osc}	λ/[nm]
imidazole (gas phase)				
S_1	$\pi\sigma^*_{NH}$	5.56	$7.77\cdot10^{-4}$	223.0
S_2	$n\sigma^*_{NH}$	6.31	$1.59\cdot10^{-2}$	196.4
S_3	$\pi\sigma^*$	6.33	$3.67\cdot10^{-2}$	195.8
S_4	$\pi\pi^*$	6.52	0.167	190.2
S_5	$\pi\sigma^*$	6.58	$1.63\cdot10^{-4}$	188.4
imidazole–$(H_2O)_5$ cluster				
S_1	$\pi\sigma^*_{NH}$	5.50	$3.55\cdot10^{-3}$	225.4
S_2	$\pi\sigma^*$	5.89	$2.47\cdot10^{-2}$	210.5
S_3	$\pi\pi^*(\pi-3s)$	6.10	$8.64\cdot10^{-2}$	203.4
S_4	$\sigma\sigma^*$	6.23	$1.37\cdot10^{-2}$	199.0
S_5	$\pi\sigma^*$	6.30	$9.23\cdot10^{-5}$	196.8
adenine (gas phase)				
S_1	$n\pi^*$	5.09	$2.67\cdot10^{-3}$	243.7
S_2	$\pi\pi^*$	5.19	0.239	238.9
S_3	$\pi\pi^*$	5.25	$6.39\cdot10^{-2}$	236.1
S_4	$\pi\sigma^*_{NH}$	5.36	$1.03\cdot10^{-2}$	231.5
S_5	$\pi\sigma^*$	5.67	$1.21\cdot10^{-3}$	218.7
adenine–$(H_2O)_5$ cluster				
S_1	$n\pi^*$	5.07	$7.95\cdot10^{-3}$	244.4
S_2	$\pi\sigma^*$	5.15	$8.61\cdot10^{-2}$	240.7
S_3	$\pi\pi^*$	5.22	0.192	237.5
S_4	$\pi\pi^*$	5.25	$3.23\cdot10^{-2}$	236.2
S_5	$\pi\sigma^*_{NH}$	5.49	$1.48\cdot10^{-3}$	226.0