Electronic Supplementary Material (ESI) for RSC Advances.

Solvent effects on the excited state characteristics of adenine-thymine base pairs†

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Supplementary materials

Table 1 Excitation energies (ΔE, eV), Oscillator strengths (f) and statistical descriptors (e.g., Ω, POS, PR, CT and COH, see the text for details) for the first 20 excited states of AT-S in solution with a constrained base pair structure with fixed gas phase geometry.

state	dE(eV)	f	Om	POS	PR	CT	COH
S_1	5.225	0.042	0.887	1.774	1.529	0.273	1.357
S_2	5.426	0.199	0.880	1.126	1.285	0.099	1.122
S_3	5.475	0.032	0.798	1.046	1.097	0.088	1.096
S_4	5.536	0.031	0.879	1.349	1.662	0.428	1.584
S_5	5.690	0.044	0.905	1.345	1.682	0.418	1.596
S_6	5.703	0.005	0.803	1.934	1.145	0.128	1.134
S_7	6.035	0.002	0.826	1.060	1.128	0.113	1.126
S_8	6.407	0.053	0.801	1.832	1.400	0.318	1.316
S_9	6.512	0.003	0.798	1.027	1.056	0.052	1.054
S_{10}	6.552	0.002	0.922	1.490	1.069	0.937	1.067
S_{11}	6.688	0.216	0.850	1.197	1.463	0.374	1.363
S_{12}	6.748	0.117	0.812	1.482	1.379	0.683	1.424
S_{13}	6.769	0.058	0.826	1.574	1.221	0.816	1.194
S_{14}	7.046	0.122	0.699	1.124	1.290	0.237	1.252
S_{15}	7.056	0.025	0.751	1.031	1.065	0.061	1.063
S_{16}	7.146	0.008	0.766	1.162	1.385	0.308	1.306
S_{17}	7.181	0.074	0.736	1.110	1.243	0.114	1.143
S_{18}	7.288	0.000	0.737	1.053	1.114	0.103	1.106
S_{19}	7.304	0.007	0.753	1.972	1.057	0.054	1.057
S_{20}	7.431	0.043	0.719	1.433	1.586	0.714	1.454

Table 2 Excitation energies (ΔE, eV), Oscillator strengths (f) and statistical descriptors (e.g., Ω, POS, PR, CT and COH, see the text for details) for the first 20 excited states of AT-S in solution with a optimized base pair structure in the presence of solvent molecules.

state	dE(eV)	f	Om	POS	PR	CT	COH
S_1	4.836	0.002	0.900	1.019	1.039	0.037	1.039
S_2	4.955	0.027	0.905	1.747	1.607	0.093	1.155
S_3	5.098	0.042	0.841	1.852	1.339	0.100	1.128
S_4	5.123	0.265	0.901	1.323	1.776	0.079	1.148
S_5	5.414	0.023	0.868	1.050	1.106	0.063	1.069
S_6	5.646	0.003	0.918	1.020	1.040	0.039	1.040
S_7	5.687	0.031	0.911	1.478	1.072	0.933	1.070
S_8	6.165	0.002	0.845	1.011	1.023	0.023	1.023
S_9	6.364	0.062	0.692	1.815	1.431	0.085	1.122
S_{10}	6.370	0.218	0.776	1.329	1.789	0.233	1.468
S_{11}	6.621	0.031	0.856	1.736	1.635	0.510	1.690
S_{12}	6.664	0.038	0.835	1.709	1.687	0.558	1.675
S_{13}	6.714	0.007	0.810	1.687	1.716	0.512	1.692
S_{14}	6.824	0.018	0.783	1.528	1.649	0.582	1.664
S_{15}	6.865	0.023	0.652	1.026	1.054	0.051	1.053
S_{16}	6.886	0.002	0.660	1.159	1.365	0.185	1.255
S_{17}	6.950	0.019	0.849	1.505	1.016	0.984	1.016
S_{18}	6.970	0.130	0.719	1.658	1.817	0.212	1.435
S_{19}	7.009	0.141	0.739	1.262	1.629	0.176	1.302
S_{20}	7.223	0.001	0.812	1.091	1.209	0.175	1.175

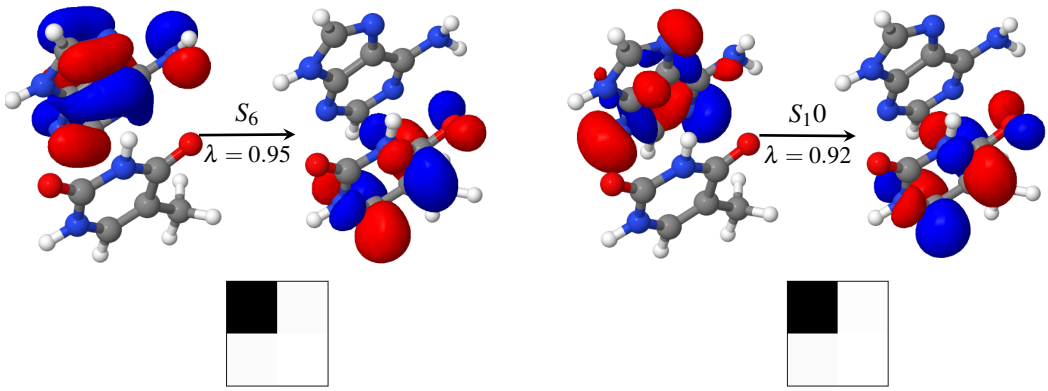

Figure 1 Charge transfer states of AT-S in gas phase (a) and in solution with a constrained base pair structure with fixed gas phase geometry (b). The symbol above the arrow identifies the singlet excited state described by the NTO pairs presented in the figure. The panel left of the arrow shows the hole density and the panel right of the arrow shows the particle density. The symbol λ bellow the arrow gives the weight of the respective configuration. Electron-hole correlation plots (Ω matrix) of the charge transfer excitation states are presented at the bottom of each figures. Ω matrix is a 2×2 matrix here as the AT dimer is divided into two fragments. Adenine and thymine is defined as fragment 1 and 2, respectively.

Table 3 Excitation energies (ΔE, eV), Oscillator strengths (f) and statistical descriptors (e.g., Ω, POS, PR, CT and COH, see the text for details) for the first 20 excited states of AT-WC in solution with a constrained base pair structure with fixed gas phase geometry.

state	dE(eV)	f	Om	POS	PR	CT	COH
S_1	5.349	0.161	0.932	1.928	1.154	0.005	1.006
S_2	5.385	0.191	0.902	1.119	1.267	0.057	1.071
S_3	5.686	0.002	0.872	1.007	1.015	0.015	1.015
S_4	5.749	0.062	0.859	1.021	1.043	0.041	1.041
S_5	5.809	0.000	0.900	1.984	1.032	0.031	1.032
S_6	6.339	0.002	0.865	1.007	1.014	0.014	1.014
S_7	6.603	0.289	0.803	1.777	1.531	0.090	1.142
S_8	6.624	0.065	0.831	1.295	1.712	0.030	1.052
S_9	6.806	0.300	0.751	1.103	1.226	0.048	1.057
S_{10}	6.821	0.062	0.820	1.851	1.341	0.029	1.038
S_{11}	7.072	0.167	0.774	1.021	1.043	0.041	1.041
S_{12}	7.319	0.104	0.743	1.034	1.073	0.068	1.068
S_{13}	7.354	0.016	0.785	1.019	1.038	0.037	1.037
S_{14}	7.479	0.234	0.815	1.996	1.008	0.008	1.008
S_{15}	7.558	0.083	0.678	1.009	1.019	0.018	1.019
S_{16}	7.634	0.042	0.708	1.039	1.083	0.077	1.077
S_{17}	7.884	0.005	0.815	1.978	1.046	0.044	1.044
S_{18}	8.059	0.001	0.859	1.895	1.233	0.190	1.226
S_{19}	8.097	0.000	0.939	1.531	1.079	0.934	1.066
S_{20}	8.159	0.004	0.799	1.140	1.324	0.252	1.298

Table 4 Excitation energies (ΔE, eV), Oscillator strengths (f) and statistical descriptors (e.g., Ω, POS, PR, CT and COH, see the text for details) for the first 20 excited states of AT-WC in solution with a optimized base pair structure in the presence of solvent molecules.

state	dE(eV)	f	Om	POS	PR	CT	COH
S_1	4.834	0.001	0.919	1.011	1.021	0.021	1.021
S_2	4.980	0.003	0.917	1.992	1.016	0.016	1.016
S_3	4.992	0.172	0.924	2.000	1.001	0.001	1.001
S_4	5.133	0.289	0.882	1.001	1.003	0.003	1.003
S_5	5.490	0.020	0.870	1.018	1.038	0.037	1.037
S_6	5.528	0.001	0.893	1.024	1.050	0.048	1.048
S_7	6.237	0.003	0.922	1.029	1.059	0.057	1.061
S_8	6.322	0.000	0.857	1.987	1.027	0.026	1.026
S_9	6.480	0.412	0.861	1.014	1.028	0.028	1.028
S_{10}	6.542	0.005	0.958	1.500	1.001	0.999	1.001
S_{11}	6.654	0.064	0.918	1.996	1.008	0.008	1.008
S_{12}	6.810	0.006	0.880	1.032	1.066	0.062	1.065
S_{13}	6.897	0.190	0.944	1.996	1.009	0.008	1.008
S_{14}	6.908	0.049	0.942	1.995	1.010	0.010	1.010
S_{15}	7.025	0.045	0.734	1.078	1.178	0.155	1.151
S_{16}	7.031	0.022	0.711	1.060	1.135	0.121	1.119
S_{17}	7.104	0.128	0.809	1.007	1.015	0.014	1.015
S_{18}	7.136	0.010	0.774	1.052	1.111	0.101	1.112
S_{19}	7.235	0.001	0.949	1.611	1.265	0.777	1.210
S_{20}	7.419	0.001	0.910	1.866	1.323	0.268	1.245