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Addition/Correction

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Correction to Pathways for Fluorescence Quenching in 2-Aminopurine π-Stacked with Pyrimidine Nucleobases

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Supporting Information

Page 6801. An error was discovered in some of the geometries used to generate the data in Table 1. These geometries were slightly distorted from the original ones causing small changes in the energies. The updated Table 1 is shown here. Whenever vertical excitations are discussed in the text, one should refer to the updated values in Table 1 in place of the old ones. As a result, the redshifts of the S_1 energy going from the monomer to the dimers given on page 6802 for 5′-2APC-3′, 5′-2APT-3′, 5′-C2AP-3′, and 5′-T2AP-3′ change from 0.08, 0.08, 0.04, 0.03 eV to 0.12, 0.07, 0.04, 0.03 eV, respectively. These changes are insignificant. The wrong initial geometries were also used as the initial point in some linear interpolation paths, so these paths are slightly changed as well. The corrected pathways are also shown here (original pathways are shown in Figures 3 and 6 of the publication), and they look almost identical to the originals. Finally, the Methods Section states incorrectly that the S_1 excited-state minimum of 2AP was optimized at the CIS(2)/cc-pVDZ+diff level, while in actuality it was optimized at the CIS(2)/cc-pVDZ level. The discussion and conclusions of the paper do not change in any way because of these corrections.

Table 1. Corrected Vertical Excitation Energies (E in eV) and Oscillator Strengths (f) of the Monomers and Dimers Studied in This Work Calculated at the CIS(2X)/cc-pvdz+diff Level

		2AP	T	C	5′-2APT-3′	5′-T2AP-3′	5′-2APC-3′	5′-C2AP-3′
S_1	E	4.79	5.12	5.07	4.72	4.76	4.67	4.75
	f	0.1992	0.0000	0.0653	0.1639	0.1551	0.1676	0.1500
S_2	E	5.07	5.68	5.42	5.02	5.01	4.99	5.05
	f	0.0039	0.2839	0.0018	0.0002	0.0043	0.0049	0.0127
S_3	E	5.70	6.16	5.88	5.05	5.12	5.02	5.06
	f	0.0032	0.0011	0.0001	0.0043	0.0000	0.0522	0.0582
S_4	E	6.01	6.62	5.92	5.45	5.64	5.33	5.43
	f	0.0123	0.0000	0.0071	0.0097	0.2296	0.0012	0.0025
S_5	E	6.01	6.91	6.08	5.60	5.69	5.34	5.58
	f	0.1423	0.0617	0.2314	0.1632	0.0056	0.0021	0.0006
S_6	E	6.55	7.07	6.14	5.86	5.89	5.71	5.76
	f	0.0034	0.0023	0.0000	0.0137	0.0335	0.0073	0.0189
S_7	E	6.56	7.17	6.44	5.94	5.98	5.78	5.83
	f	0.0014	0.1287	0.0083	0.1004	0.1209	0.0445	0.0044

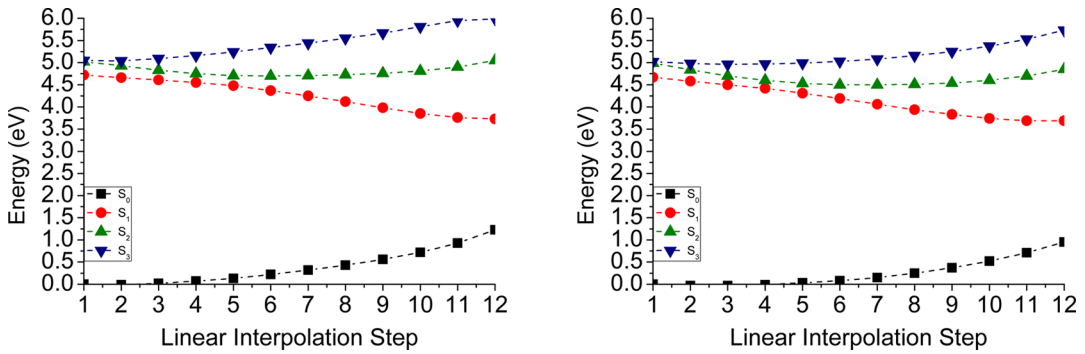

Figure 3. Energies of the S_0, S_1, S_2, S_3 excited states along the LIIC connecting the FC point to the S_1(2APB) for 5′-2APT-3′ (left panel) and 5′-2APC-3′ (right panel). Corrected Figure 3 from the original publication.

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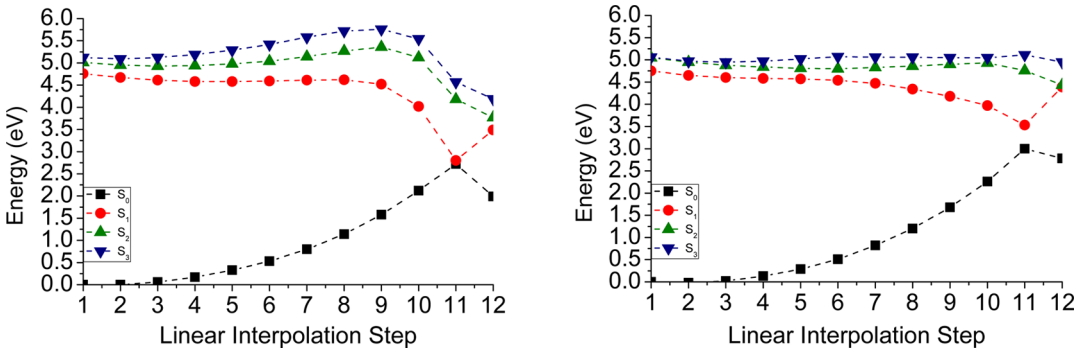

Figure 6. Energies of the S_0, S_1, S_2, S_3 excited states along the LIIC connecting the FC point to the CI for 5′-T2AP-3′ (left panel) and 5′-C2AP-3′ (right panel). Corrected Figure 6 from the original publication.

■ ASSOCIATED CONTENT

Supporting Information

Figures of LIICs between S_1(2AP) and S_1(2APB) or CI are included. Figures of the magnitude of the dipole moment change for S_1 along the LIIC connecting the FC point to the S_1(2APB) for 5′-2APT-3′ and 5′-2APC-3′ are also included. Cartesian coordinates and energies in Hartree of the geometries considered here are given. This material is available free of charge via the Internet at http://pubs.acs.org.

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