Supporting Information for
"Natural Charge-Transfer Analysis: Eliminating Spurious
Charge-Transfer States in Time-Dependent Density Functional
Theory via Diabatization, with Application to Projection-Based
Embedding"

Kevin Carter-Fenk, Christopher J. Mundy, and John M. Herbert

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Table S1: Percentage of lowest-lying CT orbital in $C_3H_4O(H_2O)_{24}$, by water molecule.[a]

Water Molecule	B3LYP			SCAN			PBE		
	SVP	TZVP	QZVP	SVP	TZVP	QZVP	SVP	TZVP	QZVP
12	52.5	64.5	66.0	62.8	65.7	64.4	65.1	67.5	66.6
4	25.6	27.3	25.9	26.4	25.9	27.3	25.8	25.2	26.1
16	4.4	4.4	4.8	5.0	5.0	5.1	4.3	4.3	4.5
13	8.6	1.9	1.3	3.7	1.6	1.4	2.9	1.3	1.1
3	1.0	0.8	0.9	0.7	0.7	0.7	0.7	0.7	0.7
21	0.4	0.6	0.6	0.5	0.6	0.6	0.4	0.6	0.6
22	0.3	0.2	0.3	0.3	0.3	0.3	0.3	0.2	0.3
11	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
19	3.0	0.1	0.1	0.2	—	—	0.2	—	—
7	0.2	0.1	< 0.1	0.1	—	—	0.1	—	—
15	3.2	—	—	0.2	0.1	0.1	0.1	—	—
9	0.3	—	—	—	—	—	—	—	—
10	0.4	—	—	—	—	—	—	—	—

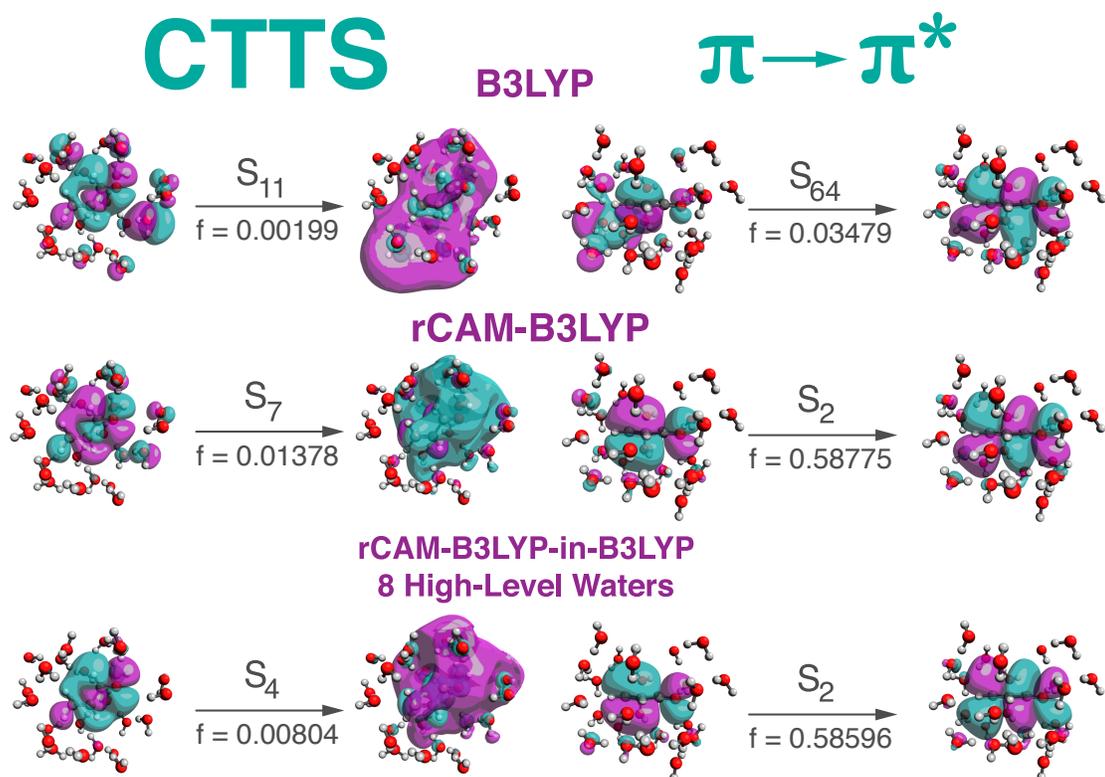[a] Karlsruhe basis, sets def2-XVP (X = S, TZ, or QZ).

Figure S1: Natural transition orbitals and oscillator strengths for the first bright CTTS state (left column) and the $\pi \rightarrow \pi^*$ transition (right column) at the (a) B3LYP, (b) rCAM-B3LYP, and (c) rCAM-B3LYP-in-B3LYP levels of theory using the jun-cc-pVDZ basis set. The embedding calculation shown features 8 high-level water molecules, as this is the lowest number of high-level waters that yields excitation energies that are converged to the canonical limit.