Analysis and Visualization of Energy Densities. II. Insights from Linear-Response Time-Dependent Density Functional Theory Calculations. **Electronic Supplementary Information**

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1 Natural Transition Orbitals

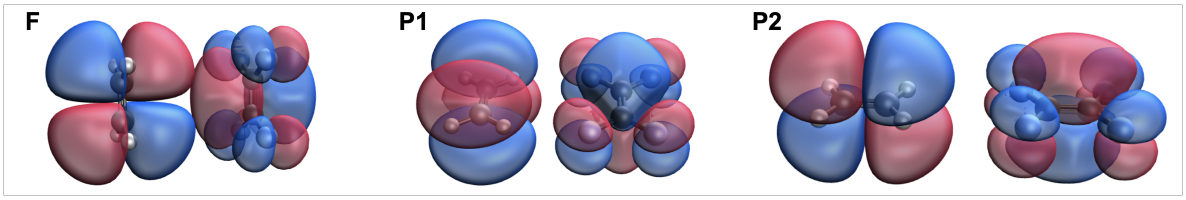

Figure S1: Natural transition orbitals of the lowest charge transfer excited-states of three C_2H_4–C_2F_4 configurations from LR-TDDFT calculations with PBE0 functional and 6-31G(d) basis set.

2 Partition Results

All charge and energy density calculations were carried out by PySCF. The only expections are FBH charges from LR-TDDFT-ωB97X-D relaxed difference densities, which were obtained from Q-Chem calculations.

In Tables S1–S9, the Tozer Λ factor, overlap between attachment and detachment density matrices (S_{DA}), fragment-based Hirshfeld partitions of excited-state charge ($\mathrm{Q}_{\mathrm{FBH}}$) and excitation energy density (kinetic $\omega_{\mathrm{FBH,T}}$ and total ω_{FBH}), and excitation energy (ω) were listed.

Table S1: LR-TDDFT Results of C_2H_4–C_2F_4 **F** configuration using the PBE functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.058	0.018	−0.998	0.998	34.908	−69.401	−0.415	5.425	5.009
	2	0.625	0.630	0.001	−0.001	−0.037	13.541	0.002	6.788	6.790
	3	0.060	0.035	0.998	−0.998	−28.689	69.786	6.411	0.403	6.814
	4	0.017	0.021	0.998	−0.998	−28.675	83.322	6.401	1.155	7.556
	5	0.024	0.018	−0.999	0.999	25.113	−69.385	2.665	5.414	8.078
6-31+G(d)	1	0.102	0.058	−0.963	0.963	28.829	−67.045	−1.048	6.190	5.142
	2	0.394	0.377	−0.209	0.209	1.569	−55.080	0.035	5.630	5.664
	3	0.546	0.528	−0.062	0.062	0.330	−18.787	0.079	6.120	6.198
	4	0.212	0.207	0.797	−0.797	−26.583	14.795	6.811	−0.549	6.262
	5	0.347	0.312	−0.460	0.460	3.816	−55.659	0.254	6.203	6.456
6-311G(d,p)	1	0.084	0.029	−0.995	0.995	34.292	−69.792	−0.832	5.859	5.028
	2	0.092	0.056	0.993	−0.993	−28.789	70.380	6.734	−0.010	6.725
	3	0.625	0.629	0.000	0.000	−0.045	12.413	0.012	6.727	6.739
	4	0.096	0.078	−0.981	0.981	16.717	−69.312	1.135	5.870	7.006
	5	0.035	0.044	0.993	−0.993	−28.751	82.549	6.716	0.682	7.398
6-311++G(d,p)	1	0.101	0.056	−0.967	0.967	29.608	−67.861	−1.160	6.283	5.123
	2	0.360	0.335	−0.383	0.384	2.561	−58.752	−0.145	5.790	5.644
	3	0.534	0.504	−0.152	0.152	0.761	−24.058	0.055	6.153	6.207
	4	0.236	0.315	0.522	−0.522	−23.291	5.039	6.119	0.120	6.239
	5	0.254	0.327	−0.485	0.486	1.792	−55.009	0.595	5.671	6.266
cc-pVDZ	1	0.069	0.025	−0.997	0.997	34.188	−69.392	−0.700	5.596	4.895
	2	0.626	0.630	0.001	−0.001	−0.045	12.748	0.004	6.763	6.767
	3	0.074	0.054	0.995	−0.995	−28.522	70.053	6.630	0.236	6.866
	4	0.053	0.044	−0.994	0.994	20.026	−69.248	1.650	5.595	7.245
	5	0.026	0.032	0.996	−0.996	−28.513	82.537	6.616	0.963	7.578
aug-cc-pVDZ	1	0.088	0.056	−0.965	0.965	29.155	−66.769	−1.150	6.147	4.996
	2	0.344	0.320	−0.395	0.395	2.503	−58.731	−0.173	5.657	5.483
	3	0.484	0.438	−0.243	0.243	1.193	−35.561	0.055	6.030	6.084
	4	0.257	0.267	−0.577	0.577	3.875	−60.548	−0.018	6.113	6.095
	5	0.259	0.213	−0.603	0.603	3.795	−61.371	0.056	6.114	6.170
cc-pVTZ	1	0.082	0.034	−0.989	0.989	32.966	−68.558	−0.968	5.936	4.969
	2	0.623	0.626	−0.001	0.001	−0.026	10.717	0.014	6.686	6.701
	3	0.090	0.067	0.987	−0.987	−28.524	69.541	6.806	−0.051	6.755
	4	0.138	0.107	−0.962	0.962	15.478	−67.578	0.953	5.950	6.904
	5	0.037	0.044	0.989	−0.989	−28.510	79.898	6.793	0.586	7.379
aug-cc-pVTZ	1	0.086	0.055	−0.966	0.966	29.365	−67.372	−1.173	6.158	4.986
	2	0.340	0.317	−0.379	0.379	2.307	−59.421	−0.183	5.649	5.466
	3	0.240	0.244	−0.596	0.596	3.806	−62.127	−0.065	6.123	6.058
	4	0.464	0.414	−0.272	0.272	1.234	−39.149	0.030	6.040	6.070
	5	0.246	0.206	−0.585	0.585	3.424	−62.254	0.014	6.124	6.138

Table S2: LR-TDDFT Results of C_2H_4–C_2F_4 **F** configuration using the PBE0 functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.092	0.042	−0.997	0.997	32.978	−66.021	0.315	6.698	7.012
	2	0.623	0.631	0.000	0.000	−0.012	15.975	−0.003	7.129	7.125
	3	0.163	0.311	0.930	−0.930	−26.069	61.985	7.274	0.952	8.226
	4	0.787	0.949	0.067	−0.067	1.570	4.361	7.691	0.715	8.406
	5	0.534	0.586	0.001	−0.001	5.829	0.029	8.497	0.010	8.508
6-31+G(d)	1	0.361	0.409	−0.134	0.134	0.816	−50.094	0.086	6.361	6.447
	2	0.437	0.575	−0.022	0.022	0.085	−4.582	0.037	6.668	6.705
	3	0.162	0.164	−0.867	0.867	21.596	−61.994	−0.438	7.284	6.845
	4	0.243	0.322	0.474	−0.474	−22.956	6.358	7.327	−0.204	7.123
	5	0.276	0.419	−0.271	0.271	4.284	−44.913	0.516	6.997	7.512
6-311G(d,p)	1	0.134	0.067	−0.992	0.992	32.028	−66.135	−0.095	7.067	6.972
	2	0.620	0.630	0.000	0.000	−0.015	14.972	−0.001	7.077	7.075
	3	0.590	0.776	0.416	−0.416	−10.663	27.598	7.671	0.388	8.059
	4	0.353	0.645	0.575	−0.575	−14.922	39.095	7.789	0.407	8.195
	5	0.550	0.631	0.002	−0.002	4.692	0.065	8.219	0.019	8.238
6-311++G(d,p)	1	0.302	0.405	−0.179	0.179	0.894	−51.070	0.047	6.432	6.479
	2	0.368	0.579	−0.025	0.025	0.083	−3.867	0.026	6.702	6.728
	3	0.171	0.158	−0.883	0.883	22.745	−62.888	−0.530	7.377	6.847
	4	0.252	0.310	0.240	−0.240	−22.340	2.446	6.969	−0.071	6.898
	5	0.287	0.210	−0.694	0.694	3.955	−60.926	−0.051	7.482	7.430
cc-pVDZ	1	0.109	0.056	−0.995	0.995	32.109	−65.978	0.035	6.856	6.890
	2	0.623	0.630	0.001	−0.001	−0.018	15.292	−0.004	7.105	7.100
	3	0.624	0.827	0.350	−0.350	−8.292	23.025	7.664	0.514	8.177
	4	0.551	0.608	0.001	−0.001	5.371	0.048	8.259	0.016	8.275
	5	0.298	0.600	0.644	−0.644	−16.787	43.557	7.732	0.573	8.305
aug-cc-pVDZ	1	0.278	0.392	−0.187	0.188	0.966	−51.489	0.010	6.321	6.330
	2	0.338	0.555	−0.039	0.039	0.133	−9.783	0.033	6.644	6.677
	3	0.136	0.158	−0.857	0.857	21.499	−61.909	−0.511	7.216	6.704
	4	0.247	0.308	0.236	−0.236	−22.580	2.201	6.939	−0.096	6.843
	5	0.280	0.202	−0.675	0.675	3.489	−60.481	−0.125	7.357	7.231
cc-pVTZ	1	0.120	0.073	−0.985	0.985	30.348	−64.971	−0.251	7.090	6.839
	2	0.614	0.627	0.000	0.000	−0.009	13.710	0.002	7.040	7.043
	3	0.818	0.911	0.075	−0.075	−1.800	4.493	7.737	0.192	7.929
	4	0.554	0.614	0.004	−0.004	3.550	0.085	8.104	0.026	8.130
	5	0.366	0.394	−0.001	0.001	−12.073	−0.715	8.007	0.169	8.177
aug-cc-pVTZ	1	0.268	0.383	−0.184	0.184	0.898	−52.434	−0.007	6.302	6.295
	2	0.319	0.545	−0.046	0.046	0.142	−11.685	0.028	6.650	6.679
	3	0.132	0.157	−0.853	0.853	21.419	−62.315	−0.530	7.211	6.682
	4	0.233	0.301	0.242	−0.242	−22.970	2.179	6.941	−0.098	6.843
	5	0.257	0.191	−0.667	0.667	3.135	−61.272	−0.162	7.339	7.177

Table S3: LR-TDDFT Results of C_2H_4–C_2F_4 **F** configuration using the ωB97X-D functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.622	0.631	0.000	0.000	−0.007	16.853	−0.003	7.178	7.175
	2	0.862	0.956	−0.007	0.007	3.955	−0.717	7.604	0.746	8.350
	3	0.534	0.578	0.001	−0.001	5.931	0.017	8.561	0.010	8.572
	4	0.815	0.939	−0.035	0.035	1.562	−5.014	0.805	7.793	8.597
	5	0.156	0.223	−0.953	0.953	31.247	−62.875	1.122	7.637	8.758
6-31+G(d)	1	0.323	0.428	−0.099	0.099	0.583	−48.302	0.097	6.701	6.797
	2	0.385	0.597	−0.013	0.013	0.047	2.353	0.022	6.843	6.864
	3	0.267	0.396	0.176	−0.176	−19.655	1.592	7.489	0.066	7.556
	4	0.715	0.831	0.040	−0.040	−7.177	−0.056	7.398	0.252	7.650
	5	0.281	0.423	−0.228	0.228	2.724	−42.921	0.137	7.693	7.830
6-311G(d,p)	1	0.616	0.631	0.000	0.000	−0.010	16.013	−0.003	7.138	7.135
	2	0.845	0.942	−0.002	0.002	2.647	−0.302	7.808	0.257	8.064
	3	0.551	0.606	0.001	−0.001	5.034	0.035	8.289	0.018	8.308
	4	0.691	0.898	−0.158	0.158	4.633	−12.355	0.355	8.171	8.527
	5	0.393	0.414	0.005	−0.005	−11.055	0.075	8.517	0.024	8.541
6-311++G(d,p)	1	0.264	0.433	−0.107	0.107	0.531	−48.761	0.094	6.727	6.821
	2	0.410	0.600	−0.012	0.012	0.038	3.105	0.016	6.868	6.883
	3	0.239	0.327	0.101	−0.101	−21.287	0.491	7.136	0.056	7.192
	4	0.608	0.844	0.039	−0.039	−6.250	0.118	7.402	0.205	7.607
	5	0.186	0.358	0.059	−0.059	−20.640	0.390	7.770	0.080	7.850
cc-pVDZ	1	0.621	0.631	0.000	0.000	−0.012	16.301	−0.005	7.165	7.160
	2	0.851	0.949	−0.007	0.007	3.066	−0.628	7.792	0.371	8.163
	3	0.551	0.594	0.001	−0.001	5.601	0.028	8.335	0.016	8.351
	4	0.595	0.864	−0.284	0.284	8.396	−19.501	0.596	7.937	8.533
	5	0.340	0.503	−0.701	0.701	23.244	−48.050	0.662	7.983	8.645
aug-cc-pVDZ	1	0.249	0.424	−0.110	0.110	0.548	−48.926	0.076	6.619	6.694
	2	0.384	0.587	−0.017	0.017	0.055	−0.550	0.022	6.846	6.867
	3	0.228	0.326	0.103	−0.103	−21.628	0.446	7.083	0.035	7.118
	4	0.632	0.813	0.024	−0.024	−6.265	−2.373	7.007	0.560	7.568
	5	0.212	0.404	−0.217	0.217	1.709	−45.764	0.461	7.174	7.635
cc-pVTZ	1	0.610	0.629	0.000	0.000	−0.007	15.296	0.000	7.127	7.127
	2	0.831	0.927	0.000	0.000	0.718	−0.224	7.694	0.209	7.903
	3	0.553	0.598	0.003	−0.003	3.937	0.050	8.185	0.025	8.211
	4	0.432	0.737	−0.488	0.488	13.691	−32.454	0.411	8.003	8.415
	5	0.371	0.403	0.007	−0.007	−11.929	0.085	8.426	0.036	8.462
aug-cc-pVTZ	1	0.215	0.406	−0.108	0.108	0.522	−50.915	0.047	6.588	6.636
	2	0.366	0.578	−0.020	0.020	0.058	−2.607	0.018	6.858	6.877
	3	0.198	0.316	0.104	−0.104	−22.292	0.474	7.082	0.031	7.113
	4	0.181	0.396	−0.203	0.203	1.021	−46.412	0.735	6.795	7.532
	5	0.570	0.789	0.028	−0.028	−5.906	−4.960	6.691	0.885	7.576

Table S4: LR-TDDFT Results of C_2H_4–C_2F_4 **P1** configuration using the PBE functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.009	0.003	−0.988	0.988	34.946	−69.454	−0.322	5.538	5.215
	2	0.009	0.004	0.988	−0.988	−28.726	69.880	6.317	0.291	6.609
	3	0.619	0.620	−0.032	0.032	0.701	10.177	0.060	6.681	6.740
	4	0.070	0.069	0.965	−0.965	−28.245	81.016	6.363	0.944	7.307
	5	0.374	0.299	−0.778	0.778	19.768	−54.261	1.892	6.266	8.158
6-31+G(d)	1	0.055	0.019	−0.974	0.974	29.339	−67.359	−0.910	6.283	5.372
	2	0.407	0.388	−0.168	0.168	1.882	−53.439	0.016	5.682	5.698
	3	0.164	0.158	0.826	−0.826	−26.415	16.721	6.683	−0.651	6.032
	4	0.533	0.510	−0.118	0.118	1.326	−24.071	−0.005	6.170	6.164
	5	0.057	0.020	0.976	−0.976	−28.075	68.546	6.660	−0.409	6.251
6-311G(d,p)	1	0.013	0.004	−0.984	0.984	34.390	−69.881	−0.708	5.975	5.267
	2	0.014	0.006	0.984	−0.984	−28.877	70.651	6.611	−0.121	6.490
	3	0.580	0.563	−0.179	0.179	3.017	−6.558	0.139	6.415	6.554
	4	0.147	0.144	0.869	−0.869	−27.010	70.083	6.707	0.311	7.018
	5	0.357	0.333	−0.706	0.706	12.591	−48.877	0.810	6.478	7.288
6-311++G(d,p)	1	0.054	0.019	−0.975	0.975	30.110	−68.141	−1.020	6.371	5.352
	2	0.395	0.370	−0.253	0.253	2.291	−55.138	−0.067	5.774	5.707
	3	0.180	0.175	0.756	−0.756	−26.486	15.921	6.699	−0.658	6.041
	4	0.526	0.491	−0.170	0.170	1.413	−29.528	−0.043	6.230	6.188
	5	0.056	0.021	0.977	−0.977	−28.458	69.241	6.749	−0.500	6.250
cc-pVDZ	1	0.009	0.003	−0.985	0.985	34.254	−69.460	−0.593	5.709	5.115
	2	0.594	0.584	−0.130	0.130	2.471	−0.595	0.148	6.477	6.625
	3	0.009	0.005	0.984	−0.984	−28.592	70.272	6.523	0.127	6.650
	4	0.128	0.126	0.902	−0.902	−27.076	73.895	6.622	0.626	7.248
	5	0.303	0.287	−0.770	0.770	16.089	−53.135	1.217	6.254	7.471
aug-cc-pVDZ	1	0.043	0.019	−0.972	0.972	29.678	−67.050	−1.031	6.237	5.205
	2	0.374	0.351	−0.271	0.271	2.232	−55.830	−0.084	5.630	5.546
	3	0.188	0.190	0.729	−0.729	−26.184	13.579	6.669	−0.641	6.028
	4	0.469	0.415	−0.309	0.309	2.118	−41.756	−0.075	6.137	6.062
	5	0.311	0.262	−0.449	0.450	2.824	−58.093	0.067	6.162	6.229
cc-pVTZ	1	0.019	0.007	−0.982	0.982	33.160	−68.675	−0.843	6.034	5.191
	2	0.558	0.532	−0.227	0.227	3.777	−14.104	0.134	6.343	6.478
	3	0.020	0.011	0.981	−0.981	−28.641	69.909	6.689	−0.147	6.542
	4	0.168	0.165	0.831	−0.831	−26.217	62.955	6.789	0.206	6.995
	5	0.452	0.438	−0.494	0.494	8.508	−34.796	0.433	6.704	7.139
aug-cc-pVTZ	1	0.042	0.019	−0.972	0.972	29.866	−67.641	−1.053	6.250	5.198
	2	0.370	0.348	−0.257	0.257	2.054	−56.759	−0.093	5.632	5.539
	3	0.181	0.183	0.742	−0.742	−26.587	13.132	6.679	−0.648	6.031
	4	0.446	0.389	−0.361	0.361	2.291	−45.315	−0.095	6.143	6.049
	5	0.296	0.251	−0.433	0.433	2.570	−59.290	0.014	6.198	6.213

Table S5: LR-TDDFT Results of C_2H_4–C_2F_4 **P1** configuration using the PBE0 functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.611	0.628	−0.010	0.010	0.194	14.812	0.026	7.074	7.099
	2	0.015	0.006	−0.990	0.990	33.109	−66.323	0.426	6.819	7.244
	3	0.015	0.018	0.990	−0.990	−28.144	66.750	7.193	0.848	8.042
	4	0.880	0.958	0.000	0.000	3.521	−0.384	7.502	0.884	8.386
	5	0.533	0.597	0.002	−0.002	5.757	0.145	8.520	−0.012	8.508
6-31+G(d)	1	0.381	0.418	−0.100	0.101	0.975	−48.722	0.057	6.420	6.476
	2	0.410	0.575	−0.040	0.040	0.409	−5.725	0.014	6.694	6.707
	3	0.207	0.258	0.597	−0.597	−23.290	10.649	7.249	−0.299	6.950
	4	0.165	0.045	−0.973	0.973	25.436	−64.514	−0.269	7.433	7.163
	5	0.295	0.393	−0.152	0.152	1.197	−43.490	0.124	7.335	7.458
6-311G(d,p)	1	0.497	0.616	−0.039	0.039	0.553	10.231	0.049	6.952	7.001
	2	0.025	0.010	−0.987	0.987	32.319	−66.575	0.048	7.191	7.239
	3	0.028	0.039	0.985	−0.985	−28.161	67.177	7.422	0.498	7.921
	4	0.250	0.397	0.308	−0.308	−16.117	17.695	7.710	0.380	8.090
	5	0.864	0.945	0.002	−0.002	2.436	−0.002	7.879	0.234	8.114
6-311++G(d,p)	1	0.359	0.417	−0.139	0.139	1.130	−48.816	0.024	6.485	6.509
	2	0.384	0.579	−0.031	0.031	0.288	−5.908	0.007	6.728	6.734
	3	0.250	0.271	0.416	−0.415	−23.203	7.259	7.068	−0.235	6.833
	4	0.245	0.047	−0.975	0.975	26.273	−65.081	−0.360	7.517	7.158
	5	0.263	0.252	0.298	−0.298	−23.019	4.821	7.460	−0.120	7.339
cc-pVDZ	1	0.545	0.621	−0.028	0.028	0.448	12.022	0.046	6.997	7.042
	2	0.014	0.007	−0.988	0.988	32.314	−66.336	0.161	6.977	7.137
	3	0.016	0.038	0.986	−0.986	−27.990	67.006	7.356	0.699	8.056
	4	0.868	0.952	0.001	−0.001	2.745	−0.077	7.851	0.366	8.217
	5	0.544	0.638	0.010	−0.010	4.930	0.612	8.271	0.001	8.273
aug-cc-pVDZ	1	0.315	0.400	−0.144	0.144	1.077	−50.225	0.010	6.352	6.362
	2	0.355	0.560	−0.053	0.053	0.459	−10.045	0.003	6.685	6.688
	3	0.202	0.280	0.377	−0.377	−23.250	5.791	7.012	−0.229	6.782
	4	0.070	0.042	−0.971	0.971	25.818	−64.230	−0.375	7.379	7.003
	5	0.211	0.330	−0.241	0.241	1.248	−50.084	0.104	7.115	7.219
cc-pVTZ	1	0.467	0.608	−0.050	0.050	0.701	7.672	0.057	6.906	6.964
	2	0.029	0.015	−0.985	0.985	30.868	−65.495	−0.103	7.197	7.095
	3	0.827	0.925	0.033	−0.033	−0.268	2.055	7.779	0.176	7.954
	4	0.251	0.371	0.328	−0.327	−16.776	15.427	7.604	0.363	7.968
	5	0.048	0.176	0.953	−0.953	−27.051	64.477	7.497	0.522	8.018
aug-cc-pVTZ	1	0.303	0.391	−0.135	0.135	0.964	−51.341	0.001	6.335	6.336
	2	0.333	0.552	−0.064	0.064	0.530	−11.115	−0.003	6.696	6.693
	3	0.189	0.272	0.381	−0.381	−23.651	5.522	7.020	−0.234	6.786
	4	0.064	0.042	−0.970	0.970	25.830	−64.605	−0.399	7.379	6.981
	5	0.191	0.312	−0.224	0.224	1.092	−51.797	0.050	7.131	7.181

Table S6: LR-TDDFT Results of C_2H_4–C_2F_4 **P1** configuration using the ωB97X-D functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.610	0.630	−0.005	0.005	0.084	16.287	0.018	7.142	7.161
	2	0.880	0.957	0.000	0.000	3.780	−0.273	7.596	0.752	8.348
	3	0.536	0.579	−0.001	0.001	5.966	−0.059	8.591	−0.019	8.572
	4	0.861	0.942	−0.001	0.001	0.384	−2.637	0.776	7.822	8.598
	5	0.018	0.015	−0.991	0.991	32.911	−66.798	1.283	7.723	9.005
6-31+G(d)	1	0.331	0.434	−0.047	0.047	0.404	−47.652	0.063	6.766	6.829
	2	0.395	0.602	−0.031	0.031	0.279	3.502	0.034	6.849	6.883
	3	0.362	0.373	0.184	−0.184	−19.147	3.108	7.491	0.066	7.557
	4	0.595	0.838	0.010	−0.010	−6.976	0.059	7.538	0.114	7.652
	5	0.258	0.445	−0.061	0.061	0.458	−37.046	0.103	7.867	7.969
6-311G(d,p)	1	0.475	0.626	−0.014	0.014	0.187	14.134	0.032	7.068	7.100
	2	0.864	0.943	0.001	−0.001	2.655	−0.061	7.854	0.214	8.068
	3	0.555	0.607	−0.001	0.001	5.100	−0.043	8.328	−0.019	8.309
	4	0.291	0.407	0.088	−0.088	−12.038	3.447	8.253	0.281	8.535
	5	0.849	0.933	−0.001	0.001	0.079	−2.768	0.230	8.313	8.543
6-311++G(d,p)	1	0.284	0.437	−0.070	0.070	0.521	−48.075	0.056	6.791	6.847
	2	0.366	0.604	−0.022	0.022	0.180	3.638	0.017	6.883	6.900
	3	0.277	0.320	0.097	−0.097	−21.501	1.453	7.180	0.043	7.222
	4	0.624	0.849	0.009	−0.009	−5.985	0.049	7.502	0.108	7.610
	5	0.191	0.253	0.096	−0.096	−21.964	0.637	7.748	0.170	7.918
cc-pVDZ	1	0.539	0.627	−0.011	0.011	0.157	14.963	0.029	7.102	7.131
	2	0.868	0.950	0.000	0.000	2.927	−0.099	7.852	0.313	8.165
	3	0.553	0.594	−0.001	0.001	5.647	−0.050	8.367	−0.017	8.350
	4	0.850	0.933	−0.001	0.001	0.129	−2.559	0.331	8.224	8.554
	5	0.016	0.018	−0.988	0.988	32.097	−66.762	1.011	7.874	8.884
aug-cc-pVDZ	1	0.233	0.423	−0.073	0.073	0.488	−48.771	0.043	6.678	6.721
	2	0.363	0.594	−0.032	0.032	0.261	1.128	0.021	6.869	6.890
	3	0.209	0.319	0.092	−0.092	−21.981	1.172	7.115	0.018	7.133
	4	0.770	0.840	0.011	−0.011	−6.489	0.059	7.461	0.109	7.571
	5	0.146	0.373	−0.126	0.126	0.448	−45.768	0.134	7.601	7.735
cc-pVTZ	1	0.444	0.623	−0.017	0.017	0.222	13.185	0.037	7.057	7.095
	2	0.851	0.929	0.001	−0.001	0.874	−0.034	7.756	0.156	7.912
	3	0.557	0.599	−0.001	0.001	4.065	−0.051	8.232	−0.018	8.214
	4	0.268	0.393	0.124	−0.124	−13.153	4.066	8.108	0.346	8.454
	5	0.839	0.924	−0.002	0.002	0.047	−2.777	0.167	8.311	8.478
aug-cc-pVTZ	1	0.201	0.407	−0.070	0.070	0.432	−50.730	0.032	6.632	6.665
	2	0.321	0.588	−0.038	0.038	0.293	−0.104	0.019	6.886	6.905
	3	0.184	0.307	0.088	−0.088	−22.717	1.019	7.107	0.013	7.120
	4	0.743	0.835	0.012	−0.012	−6.640	0.053	7.459	0.109	7.568
	5	0.123	0.336	−0.107	0.107	0.406	−49.963	0.056	7.581	7.638

Table S7: LR-TDDFT Results of C_2H_4–C_2F_4 **P2** configuration using the PBE functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.003	0.001	−0.998	0.998	34.959	−69.462	−0.339	5.491	5.151
	2	0.003	0.001	0.998	−0.998	−28.734	69.878	6.336	0.336	6.673
	3	0.625	0.629	−0.002	0.002	0.034	13.253	0.008	6.782	6.789
	4	0.013	0.015	0.997	−0.997	−28.707	83.235	6.343	1.069	7.412
	5	0.532	0.573	0.000	0.000	6.378	−0.004	8.180	−0.001	8.178
6-31+G(d)	1	0.025	0.020	−0.981	0.981	29.215	−67.335	−0.935	6.261	5.326
	2	0.411	0.393	−0.099	0.099	0.941	−53.406	0.039	5.698	5.737
	3	0.093	0.088	0.907	−0.907	−27.341	16.784	6.714	−0.603	6.111
	4	0.549	0.533	−0.048	0.048	0.416	−17.769	0.056	6.155	6.211
	5	0.011	0.005	0.990	−0.990	−28.099	68.617	6.675	−0.380	6.296
6-311G(d,p)	1	0.006	0.002	−0.996	0.996	34.408	−69.897	−0.730	5.927	5.198
	2	0.007	0.003	0.995	−0.995	−28.889	70.654	6.635	−0.075	6.560
	3	0.622	0.625	−0.014	0.014	0.204	10.885	0.030	6.694	6.724
	4	0.131	0.091	−0.943	0.943	16.150	−67.606	1.082	6.045	7.126
	5	0.032	0.036	0.986	−0.986	−28.748	81.685	6.657	0.558	7.215
6-311++G(d,p)	1	0.022	0.018	−0.982	0.982	29.994	−68.126	−1.044	6.350	5.306
	2	0.394	0.367	−0.212	0.212	1.638	−55.815	−0.054	5.810	5.756
	3	0.124	0.119	0.823	−0.823	−27.249	15.489	6.728	−0.596	6.132
	4	0.211	0.194	−0.735	0.735	5.219	−63.617	−0.136	6.348	6.212
	5	0.539	0.515	−0.113	0.113	0.721	−21.590	0.047	6.169	6.216
cc-pVDZ	1	0.004	0.002	−0.996	0.996	34.271	−69.472	−0.616	5.656	5.039
	2	0.005	0.003	0.996	−0.996	−28.603	70.270	6.547	0.179	6.727
	3	0.624	0.627	−0.008	0.008	0.135	11.758	0.022	6.735	6.757
	4	0.118	0.075	−0.964	0.964	19.492	−67.864	1.587	5.754	7.341
	5	0.027	0.032	0.990	−0.990	−28.504	81.968	6.565	0.860	7.425
aug-cc-pVDZ	1	0.022	0.019	−0.981	0.981	29.560	−67.036	−1.050	6.213	5.162
	2	0.370	0.344	−0.250	0.250	1.763	−56.331	−0.074	5.666	5.591
	3	0.208	0.196	−0.702	0.702	4.399	−62.605	−0.163	6.179	6.015
	4	0.497	0.462	−0.177	0.177	1.008	−31.372	0.063	6.045	6.108
	5	0.140	0.137	0.778	−0.778	−26.785	13.345	6.699	−0.584	6.115
cc-pVTZ	1	0.008	0.004	−0.994	0.994	33.179	−68.691	−0.860	5.999	5.139
	2	0.008	0.005	0.994	−0.994	−28.655	69.925	6.707	−0.112	6.595
	3	0.617	0.619	−0.020	0.020	0.273	8.457	0.041	6.634	6.676
	4	0.195	0.142	−0.866	0.866	14.102	−63.823	0.818	6.169	6.988
	5	0.039	0.044	0.979	−0.979	−28.458	78.380	6.740	0.452	7.191
aug-cc-pVTZ	1	0.022	0.019	−0.981	0.981	29.748	−67.627	−1.073	6.227	5.155
	2	0.365	0.341	−0.226	0.226	1.509	−57.287	−0.077	5.640	5.564
	3	0.195	0.182	−0.716	0.716	4.258	−63.702	−0.194	6.189	5.995
	4	0.131	0.127	0.796	−0.796	−27.230	12.794	6.716	−0.617	6.099
	5	0.485	0.447	−0.187	0.187	1.006	−33.877	0.038	6.068	6.107

Table S8: LR-TDDFT Results of C_2H_4–C_2F_4 **P2** configuration using the PBE0 functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.623	0.631	−0.001	0.001	0.013	15.848	0.005	7.121	7.126
	2	0.005	0.003	−0.999	0.999	33.086	−66.346	0.466	6.835	7.301
	3	0.005	0.013	0.998	−0.998	−28.154	66.736	7.274	0.948	8.222
	4	0.882	0.959	0.000	0.000	3.671	−0.238	7.819	0.580	8.399
	5	0.536	0.588	0.000	0.000	5.876	0.003	8.516	−0.001	8.515
6-31+G(d)	1	0.381	0.418	−0.048	0.048	0.380	−49.180	0.046	6.444	6.489
	2	0.454	0.577	−0.016	0.016	0.118	−4.107	0.034	6.681	6.715
	3	0.132	0.230	0.616	−0.616	−23.728	9.127	7.385	−0.213	7.172
	4	0.054	0.055	−0.954	0.954	24.172	−64.363	−0.264	7.468	7.204
	5	0.284	0.394	−0.203	0.203	1.813	−43.498	0.090	7.363	7.453
6-311G(d,p)	1	0.611	0.629	−0.004	0.004	0.046	14.459	0.014	7.055	7.069
	2	0.010	0.005	−0.996	0.997	32.292	−66.606	0.083	7.206	7.288
	3	0.069	0.280	0.921	−0.921	−25.877	62.109	7.543	0.561	8.105
	4	0.784	0.927	0.076	−0.076	0.192	5.080	7.949	0.175	8.124
	5	0.552	0.639	0.001	−0.001	4.703	0.050	8.244	0.003	8.247
6-311++G(d,p)	1	0.327	0.417	−0.072	0.072	0.467	−49.832	0.020	6.517	6.537
	2	0.355	0.579	−0.024	0.024	0.140	−3.860	0.032	6.702	6.733
	3	0.187	0.284	0.213	−0.213	−22.224	2.807	6.988	−0.068	6.920
	4	0.055	0.048	−0.960	0.960	25.209	−64.984	−0.353	7.555	7.202
	5	0.208	0.213	0.464	−0.464	−24.147	7.010	7.507	−0.167	7.341
cc-pVDZ	1	0.619	0.630	−0.002	0.002	0.033	14.943	0.011	7.086	7.097
	2	0.007	0.004	−0.997	0.997	32.286	−66.363	0.195	6.986	7.181
	3	0.829	0.945	0.044	−0.044	1.482	2.848	7.984	0.242	8.226
	4	0.037	0.224	0.954	−0.954	−26.672	64.118	7.466	0.781	8.248
	5	0.553	0.611	0.000	0.000	5.431	0.011	8.282	0.000	8.282
aug-cc-pVDZ	1	0.287	0.404	−0.085	0.085	0.516	−50.196	0.016	6.377	6.393
	2	0.305	0.557	−0.034	0.034	0.183	−9.164	0.043	6.644	6.686
	3	0.185	0.288	0.195	−0.195	−22.487	2.243	6.925	−0.077	6.848
	4	0.038	0.052	−0.953	0.953	24.564	−64.099	−0.359	7.406	7.047
	5	0.234	0.298	−0.393	0.393	2.236	−52.740	−0.084	7.241	7.157
cc-pVTZ	1	0.598	0.625	−0.006	0.006	0.068	12.886	0.021	7.009	7.031
	2	0.013	0.008	−0.995	0.995	30.827	−65.528	−0.065	7.221	7.157
	3	0.854	0.931	0.002	−0.002	0.662	0.051	7.871	0.094	7.965
	4	0.556	0.622	0.001	−0.001	3.657	0.045	8.136	0.005	8.141
	5	0.345	0.381	0.050	−0.050	−12.953	1.386	8.038	0.107	8.145
aug-cc-pVTZ	1	0.281	0.392	−0.081	0.081	0.451	−51.470	0.009	6.338	6.347
	2	0.282	0.550	−0.035	0.035	0.179	−10.509	0.034	6.659	6.693
	3	0.172	0.279	0.211	−0.211	−23.015	2.270	6.933	−0.089	6.845
	4	0.038	0.055	−0.945	0.945	24.310	−64.447	−0.383	7.404	7.022
	5	0.211	0.283	−0.400	0.400	2.103	−54.157	−0.113	7.235	7.122

Table S9: LR-TDDFT Results of C_2H_4–C_2F_4 **P2** configuration using the ωB97X-D functional.

Basis	ES#	Λ	S_{DA}	Q_{FBH} (au)		$\omega_{FBH,T}$ (eV)		ω_{FBH} (eV)		ω (eV)
				C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	
6-31G(d)	1	0.623	0.631	0.000	0.000	0.008	16.768	0.004	7.172	7.177
	2	0.882	0.958	0.000	0.000	3.918	−0.166	7.868	0.492	8.360
	3	0.536	0.579	0.000	0.000	5.973	−0.003	8.580	−0.002	8.579
	4	0.863	0.941	0.000	0.000	0.253	−2.706	0.506	8.092	8.597
	5	0.006	0.006	−0.999	0.999	32.785	−66.830	1.493	7.905	9.397
6-31+G(d)	1	0.351	0.434	−0.023	0.023	0.162	−47.723	0.043	6.773	6.815
	2	0.411	0.599	−0.007	0.007	0.052	2.727	0.023	6.851	6.873
	3	0.775	0.836	0.023	−0.023	−7.163	0.124	7.551	0.103	7.655
	4	0.242	0.405	0.066	−0.066	−17.975	0.784	7.606	0.057	7.663
	5	0.240	0.459	−0.101	0.101	0.736	−35.381	0.112	7.890	8.001
6-311G(d,p)	1	0.604	0.630	−0.002	0.002	0.020	15.735	0.009	7.123	7.132
	2	0.864	0.944	0.000	0.000	2.700	−0.037	7.948	0.128	8.076
	3	0.556	0.609	0.000	0.000	5.101	0.001	8.316	0.001	8.317
	4	0.385	0.412	0.018	−0.018	−11.188	0.426	8.444	0.088	8.532
	5	0.853	0.933	0.000	0.000	0.049	−2.701	0.134	8.415	8.549
6-311++G(d,p)	1	0.243	0.439	−0.029	0.029	0.168	−48.218	0.030	6.811	6.842
	2	0.306	0.600	−0.010	0.010	0.057	3.162	0.022	6.868	6.891
	3	0.212	0.319	0.042	−0.042	−21.221	0.349	7.156	0.035	7.191
	4	0.780	0.847	0.021	−0.021	−6.146	0.107	7.516	0.096	7.613
	5	0.175	0.340	0.055	−0.055	−20.917	0.417	7.720	0.098	7.818
cc-pVDZ	1	0.617	0.630	−0.001	0.001	0.016	16.103	0.008	7.151	7.159
	2	0.871	0.950	0.000	0.000	2.987	−0.055	7.984	0.190	8.174
	3	0.554	0.595	0.000	0.000	5.659	−0.002	8.358	0.000	8.358
	4	0.854	0.932	0.000	0.000	0.079	−2.526	0.198	8.361	8.559
	5	0.399	0.423	0.012	−0.012	−8.053	0.318	8.886	0.070	8.957
aug-cc-pVDZ	1	0.214	0.429	−0.035	0.035	0.188	−48.307	0.033	6.693	6.725
	2	0.285	0.588	−0.013	0.013	0.074	−0.225	0.030	6.847	6.877
	3	0.217	0.319	0.043	−0.043	−21.721	0.309	7.078	0.021	7.099
	4	0.759	0.838	0.022	−0.022	−6.640	0.111	7.481	0.092	7.574
	5	0.153	0.305	0.055	−0.055	−21.852	0.328	7.642	0.060	7.702
cc-pVTZ	1	0.585	0.628	−0.003	0.003	0.029	14.876	0.015	7.107	7.122
	2	0.853	0.929	0.000	0.000	0.903	−0.018	7.829	0.091	7.920
	3	0.558	0.601	0.000	0.000	4.063	0.005	8.217	0.003	8.221
	4	0.352	0.399	0.021	−0.021	−12.045	0.431	8.374	0.084	8.459
	5	0.844	0.924	0.000	0.000	0.015	−2.643	0.091	8.392	8.483
aug-cc-pVTZ	1	0.190	0.408	−0.036	0.036	0.169	−50.630	0.025	6.626	6.652
	2	0.263	0.580	−0.014	0.014	0.071	−2.047	0.025	6.863	6.888
	3	0.189	0.308	0.047	−0.047	−22.489	0.294	7.063	0.022	7.086
	4	0.707	0.834	0.024	−0.024	−6.735	0.099	7.483	0.089	7.573
	5	0.127	0.275	0.062	−0.062	−22.858	0.305	7.602	0.063	7.665

Table S10: ESP, FBH, and Becke fragment charges (Q_A), FBH and Becke fragment excitation energies (ω_A) for the lowest local excitations and charge-transfer excitations of three C_2H_4–C_2F_4 configurations. Obtained from LR-TDDFT calculations using the PBE0 functional and 6-31G(d) basis set.

Config	ES#	Q_A^{ESP} (a.u.)		Q_A^{FBH} (a.u.)		Q_A^{Becke} (a.u.)		ω_A^{FBH} (eV)		$\omega_A^{\mathrm{Becke}}$ (eV)	
		C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4
F	2	0.006	−0.006	0.000	0.000	0.000	0.000	−0.003	7.129	−0.002	7.128
P1	1	−0.041	0.041	−0.010	0.010	−0.010	0.010	0.026	7.074	0.022	7.078
P2	1	0.019	−0.019	−0.001	0.001	−0.001	0.001	0.005	7.121	0.004	7.123
F	1	−0.967	0.967	−0.997	0.997	−0.997	0.997	0.315	6.698	0.307	6.706
P1	2	−1.016	1.016	−0.990	0.990	−0.988	0.988	0.426	6.819	0.423	6.821
P2	2	−0.964	0.964	−0.999	0.999	−0.997	0.997	0.466	6.835	0.463	6.839

3 Grid-Based and Nucleus-Based Partitioning of Nuclear Attraction Energies

Two schemes were proposed by Nakai and coworkers [1] to decompose the ground-state nuclear-electron attraction energy,

$$E_A^{N,\mathrm{g}} = -\int w_A(\mathbf{r})\rho(\mathbf{r})\sum_n \frac{Z_n}{|\mathbf{r}-\mathbf{R}_n|}\,d\mathbf{r} \tag{S1}$$

$$E_A^{N,\mathrm{n}} = -\int \rho(\mathbf{r})\sum_{n\in A} \frac{Z_n}{|\mathbf{r}-\mathbf{R}_n|}\,d\mathbf{r} \tag{S2}$$

where $\rho(\mathbf{r})$ is the ground-state electron density. Ground state partitioning results for the three C_2H_4–C_2F_4 configurations are collected in Table S11, while the corresponding excited state results are tabulated in Table S12.

Table S11: Grid-based ($E_A^{N,\mathrm{g}}$) and nucleus-based ($E_A^{N,\mathrm{n}}$) partitioning of the ground-state nuclear attraction energy of three C_2H_4–C_2F_4 configurations. FBH and Becke weights, PBE functional, and 6-31G(d) basis set are used in these calculations.

Config	$E_{A,\mathrm{FBH}}^{N,\mathrm{g}}$ (a.u.)		$E_{A,\mathrm{Becke}}^{N,\mathrm{g}}$ (a.u.)		$E_A^{N,\mathrm{n}}$ (a.u.)	
	C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4
F	−325.226	−1696.137	−325.218	−1696.145	−325.110	−1696.253
P1	−329.569	−1700.528	−329.506	−1700.591	−329.616	−1700.482
P2	−315.608	−1686.667	−315.581	−1686.694	−315.651	−1686.624

Table S12: Grid-based ($\omega_A^{N,\mathrm{g}}$) and nucleus-based ($\omega_A^{N,\mathrm{n}}$) partitioning of the nuclear attraction term of excitation energies of three C_2H_4–C_2F_4 configurations. Based on Eqs. 38 and 39 of the main text. FBH and Becke weights, PBE functional, and 6-31G(d) basis set are used in these calculations.

Config	ES#	$\omega_{A,\mathrm{FBH}}^{N,\mathrm{g}}$ (eV)		$\omega_{A,\mathrm{Becke}}^{N,\mathrm{g}}$ (eV)		$\omega_A^{N,\mathrm{n}}$ (eV)	
		C_2H_4	C_2F_4	C_2H_4	C_2F_4	C_2H_4	C_2F_4
F	1 (CT)	−340.693	567.264	−340.607	567.178	−164.087	390.658
	2 (LE)	0.388	−17.173	0.383	−17.168	0.516	−17.301
	3 (CT)	350.255	−562.201	350.213	−562.158	172.697	−384.643
	4 (CT)	350.196	−584.470	350.139	−584.413	173.184	−407.458
	5 (CT)	−272.400	567.175	−272.339	567.113	−102.471	397.246
P1	1 (CT)	−344.020	568.554	−343.998	568.532	−163.225	387.759
	2 (CT)	353.910	−563.295	353.893	−563.278	172.387	−381.771
	3 (LE)	−10.111	3.085	−9.655	2.628	−4.164	−2.862
	4 (CT)	346.750	−572.338	347.100	−572.689	168.940	−394.528
	5 (CT)	−234.415	456.512	−230.434	452.530	−81.876	303.972
P2	1 (CT)	−322.475	560.521	−322.447	560.494	−171.287	409.333
	2 (CT)	330.095	−555.583	330.091	−555.579	180.098	−405.586
	3 (LE)	−0.440	−15.770	−0.417	−15.793	−0.047	−16.163
	4 (CT)	329.739	−577.428	329.755	−577.444	180.119	−427.808
	5 (LE)	−11.008	0.033	−11.055	0.080	−12.011	1.035

4 Geometry of C_2H_4–C_2F_4 Complexes

Energy values (in Hartree) and nuclear coordinates (in Å) of C_2H_4–C_2F_4 configurations, whose monomer geometries were optimized on the ωB97X-D/6-311++G(d,p) level of theory.

```
F
12
-554.0963807
C         0.6628906040    0.0000000000   -2.5000000000
C        -0.6628906040    0.0000000000   -2.5000000000
H         1.2317033864    0.9241285878   -2.5000000000
H         1.2317033864   -0.9241285878   -2.5000000000
H        -1.2317033864    0.9241285878   -2.5000000000
H        -1.2317033864   -0.9241285878   -2.5000000000
C         0.6595916614    0.0000000000    2.5000000000
C        -0.6595916614    0.0000000000    2.5000000000
F         1.3822221343    1.0961774622    2.5000000000
F         1.3822221343   -1.0961774622    2.5000000000
F        -1.3822221343   -1.0961774622    2.5000000000
F        -1.3822221343    1.0961774622    2.5000000000

P1
12
-554.0965940
C         0.6628906040   -2.5000000000    0.0000000000
C        -0.6628906040   -2.5000000000    0.0000000000
H         1.2317033864   -1.5758714122    0.0000000000
H         1.2317033864   -3.4241285878    0.0000000000
H        -1.2317033864   -1.5758714122    0.0000000000
H        -1.2317033864   -3.4241285878    0.0000000000
C         0.6595916614    2.5000000000    0.0000000000
C        -0.6595916614    2.5000000000    0.0000000000
F         1.3822221343    3.5961774622    0.0000000000
F         1.3822221343    1.4038225378    0.0000000000
F        -1.3822221343    1.4038225378    0.0000000000
F        -1.3822221343    3.5961774622    0.0000000000

P2
12
-554.0959918
C        -2.5000000000    0.0000000000    0.0000000000
C        -3.8257812080    0.0000000000    0.0000000000
H        -1.9311872176    0.9241285878    0.0000000000
H        -1.9311872176   -0.9241285878    0.0000000000
H        -4.3945939904    0.9241285878    0.0000000000
H        -4.3945939904   -0.9241285878    0.0000000000
C         3.8191833228    0.0000000000    0.0000000000
C         2.5000000000    0.0000000000    0.0000000000
F         4.5418137957    1.0961774622    0.0000000000
F         4.5418137957   -1.0961774622    0.0000000000
F         1.7773695271   -1.0961774622    0.0000000000
F         1.7773695271    1.0961774622    0.0000000000
```

5 Geometry of OLH–water Complexes

Energy values (in Hartree) and optimized nuclear coordinates (in Å) of OLH–water configurations using the ωB97X-D/6-311++G(d,p) level of theory.

```
HB1
 25
```

```
 -1517.3893302
 O         4.2538611198   -1.7102968078   -0.1350976023
 C         3.3964102437   -0.8640460222   -0.0859406977
 N         2.0273555376   -1.1458831479   -0.0973289914
 C         1.3242793726   -0.0708136003   -0.0278193880
 S         2.1176375128    1.4902628698    0.0622830011
 C         3.7077245615    0.6328554136   -0.0052917195
 H         4.3138184598    0.8368822411    0.8777987212
 H         4.2834701088    0.9340393659   -0.8810678458
 C        -0.1353073011   -0.1142940247   -0.0213642704
 S        -0.9789467739   -1.6479280033   -0.1202116923
 N        -0.8653056269    0.9466227640    0.0560134334
 C        -3.7741242270   -1.2532458443   -0.0762464236
 C        -2.4713989033   -0.7633500956   -0.0506952797
 C        -2.1987357592    0.6160598787    0.0430297164
 C        -3.2599006526    1.5252024173    0.1151242163
 C        -4.5510605475    1.0484584333    0.0915766709
 C        -4.8070093427   -0.3337940158   -0.0042851212
 O        -6.0716069925   -0.8218348565   -0.0301146719
 H        -3.9986916083   -2.3094071051   -0.1498797088
 H        -3.0518198573    2.5854334539    0.1897401919
 H        -5.3849462344    1.7411819787    0.1483214212
 H        -6.7047270793   -0.1045243627    0.0268935355
 O         6.6343604358   -0.2168495670    0.1563320983
 H         6.0017953469   -0.9397810477    0.0343875855
 H         7.4890590282   -0.6323942618    0.2664158559

HB2
 25
 -1517.3851365
 O         5.0259513484   -2.0014583322   -0.0316786647
 C         4.2870055691   -1.0599050082   -0.0195902268
 N         2.8819536360   -1.1520773836   -0.0226945452
 C         2.3299593991    0.0045091464   -0.0092913001
 S         3.3252712664    1.4573053635    0.0102155570
 C         4.7872245795    0.3941181819    0.0016537620
 H         5.3923123267    0.5531723007    0.8943126994
 H         5.4005646549    0.5775573914   -0.8805935767
 C         0.8766259455    0.1614966296   -0.0095077730
 S        -0.1660211427   -1.2461002185   -0.0233549430
 N         0.2997054642    1.3153765189    0.0013697439
 C        -2.8810978010   -0.4791167950   -0.0178181022
 C        -1.5241528495   -0.1649122829   -0.0148740276
 C        -1.0672891776    1.1677582022   -0.0013652846
 C        -1.9937927795    2.2153360921    0.0095735641
 C        -3.3381914072    1.9163637961    0.0038500803
 C        -3.7720016050    0.5786566290   -0.0106176172
 O        -5.1051569251    0.2750575801   -0.0211521256
 H        -3.2505920093   -1.4982578426   -0.0204390721
 H        -1.6431137918    3.2398060457    0.0209210291
 H        -4.0705213241    2.7177214825    0.0090674630
 H        -5.6308461690    1.0720591820    0.0620210063
 O        -5.3641244758   -2.6073825078    0.1204771076
 H        -5.5810960020   -1.6704576957    0.0619820363
 H        -5.9193651539   -3.0449055372   -0.5245561629

T1.6
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 -1517.3649052
 O        -4.7930287203    1.5941094205    0.1280499006
 C        -3.9435865972    0.7517553082    0.0922975267
 N        -2.5601893057    1.0176468787    0.0884265343
 C        -1.8707695535   -0.0622449643    0.0490702525
 S        -2.6766812938   -1.6253285409    0.0057999983
 C        -4.2597126006   -0.7518015777    0.0466498860
 H        -4.8347924661   -1.0267494424    0.9309521335
 H        -4.8500930330   -0.9697932719   -0.8433737380
 C        -0.4091348319   -0.0346182506    0.0421194685
```

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 S         0.4458955352    1.4974835522    0.0859023645
 N         0.3117963693   -1.1019367688    0.0037510161
 C         3.2400505115    1.0788022798    0.1056610113
 C         1.9303205691    0.5999987520    0.0505104515
 C         1.6470148267   -0.7821615018    0.0093919767
 C         2.7030881473   -1.7026849679    0.0265958224
 C         3.9993285342   -1.2368589283    0.0790654603
 C         4.2691419939    0.1478199993    0.1184032553
 O         5.5302595850    0.6256924374    0.2038209922
 H         3.4719340383    2.1337511749    0.1712485626
 H         2.4864778886   -2.7629689814    0.0354238488
 H         4.8231418407   -1.9400358178    0.1341814217
 H         6.1520619473   -0.0953473168    0.3166390784
 H         2.9196211740   -0.3555486229    1.6841345732
 O         2.9124016296   -0.4777833107    2.6509028988
 H         2.5461490113    0.3323871612    3.0054092039

T1.7
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 -1517.3702160
 O        -4.7955588337    1.5942681066    0.1207736146
 C        -3.9458103010    0.7521828067    0.0863554274
 N        -2.5624496420    1.0185782990    0.0841115317
 C        -1.8726395865   -0.0610205586    0.0451429217
 S        -2.6779774173   -1.6244548722    0.0013729286
 C        -4.2613459832   -0.7514966895    0.0409266175
 H        -4.8366808273   -1.0263481110    0.9251138257
 H        -4.8513161715   -0.9700489235   -0.8492154203
 C        -0.4109046876   -0.0332429320    0.0384745670
 S         0.4445454891    1.4984717655    0.0825523376
 N         0.3095831484   -1.1008504576    0.0005495449
 C         3.2383471771    1.0788304120    0.0953702795
 C         1.9289818219    0.6001947097    0.0475609229
 C         1.6453788987   -0.7812954558    0.0065322078
 C         2.7004751955   -1.7019662586    0.0171444854
 C         3.9967404977   -1.2364029162    0.0633689901
 C         4.2667675921    0.1477671107    0.1008820777
 O         5.5293404089    0.6254821159    0.1710477277
 H         3.4710188436    2.1340491245    0.1541219872
 H         2.4836859210   -2.7623211380    0.0206186998
 H         4.8214125529   -1.9394843362    0.1076784087
 H         6.1524277850   -0.0958209687    0.2745542877
 H         2.9359488118   -0.3568752410    1.7696232561
 O         2.9281144718   -0.4808407006    2.7320471916
 H         2.5526100347    0.3262298088    3.0843254814

T1.8
 25
 -1517.3742191
 O        -4.7968532131    1.5949258404    0.1184197734
 C        -3.9470461237    0.7529597990    0.0831815456
 N        -2.5636671113    1.0195929632    0.0795659686
 C        -1.8737668599   -0.0599096642    0.0406064958
 S        -2.6789034001   -1.6234927394   -0.0018750736
 C        -4.2623927878   -0.7507682652    0.0379376727
 H        -4.8376114015   -1.0256645487    0.9221717339
 H        -4.8523929855   -0.9694168588   -0.8521716536
 C        -0.4119345297   -0.0321278506    0.0329180485
 S         0.4438482500    1.4994007964    0.0753794164
 N         0.3082052793   -1.0999611371   -0.0037577130
 C         3.2375880945    1.0788138977    0.0827550972
 C         1.9284288743    0.6005242826    0.0412740847
 C         1.6444866690   -0.7806061013    0.0017438672
 C         2.6988852950   -1.7014426106    0.0059827358
 C         3.9953652089   -1.2362025678    0.0464164310
 C         4.2654634735    0.1476094486    0.0834800627
 O         5.5289781579    0.6253587424    0.1410915681
 H         3.4710305073    2.1342166627    0.1353732787
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 H         2.4817554629   -2.7618207042    0.0044147170
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 H         6.1526408892   -0.0953523035    0.2452023944
 H         2.9476613567   -0.3688964003    1.8538059641
 O         2.9455946340   -0.4779137081    2.8149313048
 H         2.5446824240    0.3230856804    3.1531762590

T1.9
 25
 -1517.3771603
 O        -4.7968675731    1.5969244894    0.1115908846
 C        -3.9471539640    0.7547940529    0.0781467068
 N        -2.5637400985    1.0212339032    0.0752939694
 C        -1.8739343005   -0.0583532008    0.0375620770
 S        -2.6793094404   -1.6219163055   -0.0037176884
 C        -4.2626778889   -0.7489462961    0.0348870850
 H        -4.8378797157   -1.0225625729    0.9195481137
 H        -4.8528097419   -0.9688068439   -0.8548252038
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 O         5.5292886489    0.6262094931    0.1093128494
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 H         2.5197448310    0.3107409384    3.2219053837

T2.0
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 O        -4.7958109488    1.5994521710    0.1159949457
 C        -3.9465898952    0.7570321045    0.0791366150
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 S        -2.6798016947   -1.6200724728   -0.0078915815
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 C        -0.4118070575   -0.0298396414    0.0262855317
 S         0.4448260510    1.5012244491    0.0657021497
 N         0.3076339244   -1.0982582224   -0.0092123827
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 H         3.4718930773    2.1355163930    0.0991483349
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 H         4.8211632324   -1.9378926706    0.0328705594
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 O         2.9744591403   -0.4574765578    2.9869204814
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T2.1
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C       -0.4067291796   -0.0262920921    0.0189812075
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O        2.9703410905   -0.4625130114    3.0658010651
H        2.3982872997    0.2588054017    3.3297943176
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References

[1] Y. Imamura, A. Takahashi and H. Nakai, Grid-based energy density analysis: Implementation and assessment, *J. Chem. Phys.*, 2007, **126**, 034103