

Supplementary Information

Pathways to Fluorescence via Restriction of Intramolecular Motion in Substituted Tetraphenylethylenes

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Table of Contents

1.	Vertical excitations for TPE and substituted TPE.	
	Table S1. Vertical excitations for TPE using the TD-LC-DFTB2 and ω B97xD approaches.....	S4
	Table S2. Vertical excitations for TPE(CN) using the TD-LC-DFTB2 and ω B97xD approaches.....	S4
	Table S3. Vertical excitations for TPE(CN) ₅ using the TD-LC-DFTB2 and ω B97xD approaches.	S5
	Table S4. Vertical excitations for TPE(CN) ₅ (OH) using the TD-LC-DFTB2 and ω B97xD approaches.	S5
	Table S5. Vertical excitations for TPE(CN) ₅ (CF ₃) using the DFTB2-halorg-0-1 and ω B97xD approaches.	S6
	Table S6. Vertical excitations for TPE(OH)(CHO) using the TD-LC-DFTB2 and ω B97xD approaches.	S6
	Table S7. Vertical excitations for TPE(OH)(COOH) using the TD-LC-DFTB2 and ω B97xD approaches.	S7
	Table S8. Vertical excitations for TPE(OH)(CONH ₂) using the TD-LC-DFTB2 and ω B97xD approaches.....	S8
	Table S9. Vertical excitations for TPE(OH) ₂ (CHO) ₂ using the TD-LC-DFTB2 and ω B97xD approaches.	S8
	Table S10. Vertical excitations for TPE(OH) ₂ (COOH) ₂ using the TD-LC-DFTB2 and ω B97xD approaches.....	S9
	Table S11. Vertical excitations for TPE(OH) ₂ (CONH ₂) ₂ using the TD-LC-DFTB2 and ω B97xD approaches.....	S9
2.	Plots of HOMOs and LUMOs, simulated spectra, and dynamics simulations for TPE and substituted TPE.	
	Figure S1. HOMO and LUMO of (a) TPE, (b) TPE(CN), (c) TPE(CN) ₅ , (d) TPE(CN) ₅ OH, and (e) TPE(CN) ₅ CF ₃ using the ω B97xD approach.....	S10
	Figure S2. Simulated spectra for group I substituted TPE compounds: a) TPE, b) TPE(CN), c) TPE(CN) ₅ , d) TPE(CN) ₅ (OH), e) TPE(CN) ₅ (CF ₃); 250 points and 10 states were calculated with TD-LC-DFTB2. Vertical lines indicate the boundaries of the window for the initial conditions of the dynamics.....	S11
	Figure S3. Simulated spectra for group II substituted TPE compounds: a) TPE(OH)(CHO), b) TPE(OH)(COOH), c) TPE(OH)(CONH ₂), d) TPE(OH) ₂ (CHO) ₂ , e) TPE(OH) ₂ (COOH) ₂ , f) TPE(OH) ₂ (CONH ₂) ₂ ; 250 points and 10 states were calculated with TD-LC-DFTB2. Vertical lines indicate the boundaries of the window for the initial conditions of the dynamics.	S11
	Figure S4. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN) ₅ (OH) using ω B97XD dynamics simulations.	

.....	S12
Figure S5. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN) ₅ (CF ₃) using ω B97XD dynamics simulations.	S12
.....	S13
Figure S6. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN) ₅ (CF ₃) using LC-DFTB dynamics simulations.	S13
.....	S13
Figure S7. Averaged values for TPE with TD-LC-DFTB2.....	S13
Figure S8. Averaged values for TPE with ω B97XD.....	S13
Figure S9. Averaged values for TPE(CN) with TD-LC-DFTB2.	S14
Figure S10. Averaged values for TPE(CN) with ω B97XD.....	S14
Figure S11. Averaged values for TPE(CN) ₅ with TD-LC-DFTB2.	S14
Figure S12. Averaged values for TPE(CN) ₅ with ω B97XD.	S15
Figure S13. Averaged values for TPE(CN) ₅ (CF ₃) with ω B97XD.	S15
Figure S14. Averaged values for TPE(CN) ₅ (CF ₃) with TD-LC-DFTB2.	S15
Figure S15. The average occupation for a) TPE, b) TPE(CN), c) TPE(CN) ₅ , d) TPE(CN) ₅ OH with TD-LC-DFTB2.....	S16
Figure S16. The average occupation for a) TPE, b) TPE(CN), c) TPE(CN) ₅ OH with ω B97XD.	S16
Figure S17. Averaged values for TPE(CN) ₅ (OH) with TD-LC-DFTB2.....	S17
Figure S18. Averaged values for TPE(CN) ₅ (OH) with ω B97XD.....	S17
Figure S19. The average occupation for a) TPE(OH)(CHO), b) TPE(OH) ₂ (CHO) ₂ , c) TPE(OH)(CONH ₂), d) TPE(OH) ₂ (CONH ₂) ₂ , e) TPE(OH)(COOH), f) TPE(OH) ₂ (COOH) ₂ with TD-LC-DFTB2.	S17
Figure S20. The average occupation for a) TPE(OH)(CHO), b) TPE(OH) ₂ (CHO) ₂ , c) TPE(OH)(CONH ₂), d) TPE(OH) ₂ (CONH ₂) ₂ , e) TPE(OH)(COOH), f) TPE(OH) ₂ (COOH) ₂ with ω B97XD.	S18
3. Cartesian Coordinates (Å) for and total energies (a.u.) for ω B97xD and TD-LC-DFTB2 in S ₀ and S ₁	S18

Table S1. Vertical excitations for TPE using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.673	0.558	H (62a) $\rightarrow$ L (63a) (1.000)
	2	5.533	0.047	H-4 $\rightarrow$ L (0.999)
	3	5.547	0.122	H-1 $\rightarrow$ L (0.999)
	4	5.600	0.255	H $\rightarrow$ L+1 (0.994)
	5	5.602	0.001	H $\rightarrow$ L+2 (0.759)
	6	5.645	0.000	H $\rightarrow$ L+3 (0.830)
	7	5.696	0.000	H $\rightarrow$ L+5 (0.815)
	8	5.727	0.008	H $\rightarrow$ L+4 (0.927)
	9	5.735	0.085	H $\rightarrow$ L+6 (0.878)
	10	5.863	0.000	H-3 $\rightarrow$ L (0.952)
ω B97xD	1	4.342	0.424	H (88a) $\rightarrow$ L (89a) (0.977)
	2	4.955	0.002	H $\rightarrow$ L+1 (0.780)
	3	5.104	0.145	H $\rightarrow$ L+2 (0.787)
	4	5.195	0.000	H $\rightarrow$ L+5 (0.561)
	5	5.284	0.000	H $\rightarrow$ L+6 (0.543)
	6	5.416	0.209	H $\rightarrow$ L+4 (0.628)
	7	5.416	0.003	H $\rightarrow$ L+3 (0.851)
	8	5.632	0.068	H-1 $\rightarrow$ L (0.769)
	9	5.866	0.083	H-4 $\rightarrow$ L (0.804)
	10	5.878	0.000	H-2 $\rightarrow$ L (0.687)

Table S2. Vertical excitations for TPE(CN) using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.687	0.324	H (70a) $\rightarrow$ L (71a) (1.000)
	2	5.152	0.028	H $\rightarrow$ L+1 (0.999)
	3	5.159	0.207	H $\rightarrow$ L+2 (0.999)
	4	5.492	0.207	H-1 $\rightarrow$ L (0.991)
	5	5.544	0.068	H $\rightarrow$ L+3 (0.809)
	6	5.566	0.019	H $\rightarrow$ L+4 (0.757)
	7	5.619	0.026	H-5 $\rightarrow$ L (0.910)
	8	5.676	0.005	H-2 $\rightarrow$ L (0.601)
	9	5.702	0.009	H $\rightarrow$ L+6 (0.736)
	10	5.748	0.036	H-3 $\rightarrow$ L (0.533)
ω B97xD	1	4.324	0.256	H (100a) $\rightarrow$ L (101a) (0.963)
	2	4.776	0.246	H $\rightarrow$ L+1 (0.888)
	3	4.787	0.013	H $\rightarrow$ L+2 (0.836)
	4	5.155	0.015	H $\rightarrow$ L+3 (0.533)

	5	5.182	0.049	H-2 $\rightarrow$ L (0.443)
	6	5.318	0.010	H $\rightarrow$ L+3 (0.505)
	7	5.366	0.094	H $\rightarrow$ L+4 (0.364)
	8	5.570	0.051	H $\rightarrow$ L+3 (0.555)
	8	5.629	0.046	H-1 $\rightarrow$ L (0.685)
	10	5.632	0.059	H-2 $\rightarrow$ L (0.547)

Table S3. Vertical excitations for TPE(CN)₅ using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.157	0.016	H (102a) $\rightarrow$ L (103a) (0.999)
	2	4.158	0.010	H $\rightarrow$ L+1 (0.999)
	3	4.254	0.183	H $\rightarrow$ L+2 (1.000)
	4	4.595	0.000	H $\rightarrow$ L+3 (0.999)
	5	4.631	0.000	H-4 $\rightarrow$ L+1 (0.619)
	6	4.632	0.009	H-4 $\rightarrow$ L (0.605)
	7	4.847	0.064	H-5 $\rightarrow$ L (0.641)
	8	4.915	0.001	H-5 $\rightarrow$ L+1 (0.708)
	9	5.037	0.003	H-3 $\rightarrow$ L (0.852)
	10	5.037	0.001	H-3 $\rightarrow$ L+1 (0.853)
ω B97xD	1	3.694	0.016	H (148a) $\rightarrow$ L (149a) (0.944)
	2	3.715	0.119	H $\rightarrow$ L+1 (0.869)
	3	3.752	0.134	H $\rightarrow$ L+2 (0.866)
	4	4.213	0.000	H $\rightarrow$ L+3 (0.913)
	5	4.377	0.017	H-1 $\rightarrow$ L+1 (0.609)
	6	4.378	0.001	H-1 $\rightarrow$ L+1 (0.646)
	7	4.539	0.003	H-1 $\rightarrow$ L+2 (0.754)
	8	4.565	0.005	H-2 $\rightarrow$ L+2 (0.738)
	9	4.605	0.038	H-2 $\rightarrow$ L+1 (0.788)
	10	4.618	0.000	H-1 $\rightarrow$ L+1 (0.476)

Table S4. Vertical excitations for TPE(CN)₅(OH) using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator strength	Configuration (coefficient)
TD-LC-DFTB2	1	3.653	0.005	H (108a) $\rightarrow$ L (109a) (0.744)
	2	3.661	0.002	H $\rightarrow$ L+1 (0.744)
	3	3.807	0.037	H $\rightarrow$ L+2 (0.999)
	4	3.936	0.000	H-1 $\rightarrow$ L (0.735)
	5	3.949	0.008	H-1 $\rightarrow$ L+1 (0.735)
	6	4.069	0.000	H-1 $\rightarrow$ L+2 (0.858)
	7	4.148	0.001	H $\rightarrow$ L+3 (0.865)

ω B97xD	8	4.395	0.015	H-1 $\rightarrow$ L+3 (0.695)
	9	4.408	0.022	H-2 $\rightarrow$ L+1 (0.719)
	10	4.418	0.005	H-1 $\rightarrow$ L+3 (0.965)
	1	3.776	0.014	H (156a) $\rightarrow$ L (157a) (0.930)
	2	3.790	0.072	H $\rightarrow$ L+1 (0.794)
	3	3.867	0.130	H $\rightarrow$ L+2 (0.799)
	4	4.255	0.005	H-2 $\rightarrow$ L (0.564)
	5	4.275	0.003	H-1 $\rightarrow$ L (0.694)
	6	4.281	0.001	H $\rightarrow$ L+3 (0.877)
	7	4.418	0.056	H-1 $\rightarrow$ L (0.590)
	8	4.424	0.000	H-1 $\rightarrow$ L+2 (0.819)
	9	4.460	0.002	H-1 $\rightarrow$ L+1 (0.620)
	10	4.479	0.001	H-2 $\rightarrow$ L+2 (0.686)

Table S5. Vertical excitations for TPE(CN)₅(CF₃) using the DFTB2-halorg-0-1 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator strength	Configuration (coefficient)
DFTB2-halorg-0-1	1	3.009	0.186	H (126a) $\rightarrow$ L (127a) (0.999)
	2	3.073	0.005	H $\rightarrow$ L+1 (1.000)
	3	3.078	0.006	H $\rightarrow$ L+2 (1.000)
	4	3.387	0.000	H $\rightarrow$ L+3 (0.995)
	5	3.497	0.001	H-1 $\rightarrow$ L (0.997)
	6	3.518	0.004	H-2 $\rightarrow$ L (1.000)
	7	3.564	0.000	H-3 $\rightarrow$ L (1.000)
	8	3.639	0.004	H-5 $\rightarrow$ L (0.953)
	9	3.643	0.002	H-1 $\rightarrow$ L+1 (0.592)
	10	3.672	0.033	H-6 $\rightarrow$ L (0.781)
ω B97xD	1	3.846	0.302	H (180a) $\rightarrow$ L (181a) (0.932)
	2	3.975	0.018	H $\rightarrow$ L+1 (0.846)
	3	4.007	0.029	H $\rightarrow$ L+2 (0.824)
	4	4.429	0.003	H $\rightarrow$ L+3 (0.699)
	5	4.553	0.015	H $\rightarrow$ L+1 (0.453)
	6	4.565	0.055	H-2 $\rightarrow$ L (0.441)
	7	4.724	0.003	H-1 $\rightarrow$ L (0.579)
	8	4.766	0.122	H-4 $\rightarrow$ L+1 (0.497)
	9	4.791	0.029	H-2 $\rightarrow$ L (0.683)
	10	4.835	0.003	H-3 $\rightarrow$ L (0.548)

Table S6. Vertical excitations for TPE(OH)(CHO) using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
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TD-LC-DFTB2	1	3.671	0.000	H-2 (76a) $\rightarrow$ L (79a) (0.816)
	2	3.680	0.003	H-2 $\rightarrow$ L+1 (0.785)
	3	4.296	0.003	H $\rightarrow$ L+1 (0.789)
	4	4.318	0.008	H $\rightarrow$ L (0.896)
	5	4.335	0.001	H-1 $\rightarrow$ L (0.973)
	6	4.346	0.005	H-1 $\rightarrow$ L+1 (0.941)
	7	4.726	0.034	H-2 $\rightarrow$ L+1 (0.827)
	8	4.760	0.026	H-2 $\rightarrow$ L (0.806)
	9	5.119	0.072	H-4 $\rightarrow$ L (0.743)
	10	5.128	0.020	H-6 $\rightarrow$ L+1 (0.680)
ω B97xD	1	3.724	0.040	H (110a) $\rightarrow$ L (111a) (0.676)
	2	3.869	0.002	H $\rightarrow$ L+1 (0.576)
	3	4.132	0.019	H $\rightarrow$ L (0.544)
	4	4.295	0.003	H $\rightarrow$ L+1 (0.520)
	5	4.376	0.022	H-1 $\rightarrow$ L (0.747)
	6	4.536	0.053	H-1 $\rightarrow$ L+1 (0.463)
	7	4.661	0.029	H-1 $\rightarrow$ L+1 (0.586)
	8	4.779	0.055	H-2 $\rightarrow$ L (0.450)
	9	4.796	0.089	H-2 $\rightarrow$ L+1 (0.496)
	10	4.996	0.007	H-8 $\rightarrow$ L (0.319)

Table S7. Vertical excitations for TPE(OH)(COOH) using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.343	0.021	H-2 (82a) $\rightarrow$ L (85a) (0.647)
	2	4.390	0.006	H-3 $\rightarrow$ L (0.546)
	3	4.641	0.010	H $\rightarrow$ L (0.893)
	4	4.718	0.008	H $\rightarrow$ L+1 (0.753)
	5	4.757	0.011	H-1 $\rightarrow$ L (0.836)
	6	4.889	0.018	H-1 $\rightarrow$ L+1 (0.725)
	7	4.988	0.123	H $\rightarrow$ L+2 (0.838)
	8	5.105	0.130	H-2 $\rightarrow$ L+1 (0.861)
	9	5.258	0.009	H $\rightarrow$ L+2 (0.770)
	10	5.335	0.009	H-2 $\rightarrow$ L (0.727)
ω B97xD	1	4.189	0.144	H (118a) $\rightarrow$ L (119a) (0.846)
	2	4.617	0.051	H $\rightarrow$ L+1 (0.774)
	3	4.692	0.084	H-1 $\rightarrow$ L+2 (0.458)
	4	4.718	0.020	H-1 $\rightarrow$ L (0.659)
	5	4.995	0.013	H-1 $\rightarrow$ L+1 (0.507)
	6	5.053	0.058	H-2 $\rightarrow$ L+2 (0.463)
	7	5.100	0.131	H-2 $\rightarrow$ L (0.606)
	8	5.186	0.007	H $\rightarrow$ L+3 (0.484)
	9	5.241	0.012	H-6 $\rightarrow$ L (0.396)

	10	5.368	0.056	H-1 $\rightarrow$ L (0.366)
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Table S8. Vertical excitations for TPE(OH)(CONH₂) using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.475	0.033	H-1 (83a) $\rightarrow$ L (85a) (0.577)
	2	4.511	0.002	H-3 $\rightarrow$ L (0.732)
	3	4.703	0.069	H $\rightarrow$ L (0.925)
	4	4.921	0.045	H $\rightarrow$ L (0.635)
	5	4.940	0.059	H $\rightarrow$ L+1 (0.792)
	6	5.052	0.096	H $\rightarrow$ L+2 (0.931)
	7	5.207	0.014	H-1 $\rightarrow$ L+1 (0.876)
	8	5.240	0.103	H-2 $\rightarrow$ L+2 (0.578)
	9	5.298	0.028	H-1 $\rightarrow$ L+2 (0.862)
	10	5.379	0.085	H-2 $\rightarrow$ L+1 (0.519)
ω B97xD	1	4.329	0.180	H (118a) $\rightarrow$ L (119a) (0.847)
	2	4.728	0.129	H $\rightarrow$ L+1 (0.705)
	3	4.763	0.023	H-1 $\rightarrow$ L+2 (0.481)
	4	4.837	0.002	H-1 $\rightarrow$ L (0.635)
	5	5.056	0.019	H-1 $\rightarrow$ L+1 (0.482)
	6	5.104	0.046	H-2 $\rightarrow$ L+2 (0.434)
	7	5.199	0.047	H $\rightarrow$ L+3 (0.465)
	8	5.206	0.010	H-6 $\rightarrow$ L (0.350)
	9	5.272	0.055	H-2 $\rightarrow$ L+1 (0.348)
	10	5.428	0.023	H-9 $\rightarrow$ L+1 (0.355)

Table S9. Vertical excitations for TPE(OH)₂(CHO)₂ using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
TD-LC-DFTB2	1	3.979	0.057	H-2 (92a) $\rightarrow$ L (95a) (0.980)
	2	4.046	0.006	H-4 $\rightarrow$ L+2 (0.627)
	3	4.076	0.028	H-4 $\rightarrow$ L+1 (0.613)
	4	4.133	0.004	H-4 $\rightarrow$ L (0.632)
	5	4.169	0.022	H-3 $\rightarrow$ L (0.663)
	6	4.339	0.006	H $\rightarrow$ L (0.864)
	7	4.353	0.007	H-1 $\rightarrow$ L (0.871)
	8	4.420	0.002	H-2 $\rightarrow$ L+1 (0.993)
	9	4.488	0.007	H-2 $\rightarrow$ L+2 (0.993)
	10	4.616	0.001	H-1 $\rightarrow$ L+1 (0.890)
ω B97xD	1	3.616	0.059	H-2 (130a) $\rightarrow$ L (133a) (0.882)
	2	3.952	0.000	H-2 $\rightarrow$ L+1 (0.516)

	3	3.998	0.010	H $\rightarrow$ L (0.755)
	4	4.034	0.005	H-1 $\rightarrow$ L (0.834)
	5	4.075	0.000	H-11 $\rightarrow$ L+1 (0.351)
	6	4.092	0.000	H-2 $\rightarrow$ L+2 (0.684)
	7	4.178	0.01	H-2 $\rightarrow$ L+1 (0.524)
	8	4.215	0.011	H-9 $\rightarrow$ L+2 (0.404)
	9	4.354	0.001	H-2 $\rightarrow$ L+2 (0.459)
	10	4.392	0.003	H $\rightarrow$ L+1 (0.795)

Table S10. Vertical excitations for TPE(OH)₂(COOH)₂ using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.154	0.151	H (106a) $\rightarrow$ L (107a) (0.949)
	2	4.424	0.058	H-1 $\rightarrow$ L (0.962)
	3	4.484	0.027	H-2 $\rightarrow$ L (0.975)
	4	4.578	0.031	H-3 $\rightarrow$ L+1 (0.792)
	5	4.660	0.002	H-3 $\rightarrow$ L (0.908)
	6	4.691	0.017	H-4 $\rightarrow$ L (0.853)
	7	4.829	0.003	H $\rightarrow$ L+1 (0.954)
	8	4.895	0.007	H-4 $\rightarrow$ L (0.862)
	9	4.973	0.001	H-6 $\rightarrow$ L (0.778)
	10	5.068	0.030	H-5 $\rightarrow$ L (0.925)
ω B97xD	1	4.080	0.125	H-1 (148a) $\rightarrow$ L (149a) (0.764)
	2	4.385	0.099	H-1 $\rightarrow$ L (0.759)
	3	4.865	0.009	H-2 $\rightarrow$ L (0.543)
	4	4.918	0.027	H-1 $\rightarrow$ L+1 (0.521)
	5	4.960	0.046	H-3 $\rightarrow$ L (0.431)
	6	5.020	0.042	H $\rightarrow$ L+1 (0.457)
	7	5.089	0.055	H $\rightarrow$ L+1 (0.462)
	8	5.099	0.065	H-5 $\rightarrow$ L (0.328)
	9	5.170	0.026	H-1 $\rightarrow$ L+2 (0.416)
	10	5.262	0.031	H-1 $\rightarrow$ L+3 (0.451)

Table S11. Vertical excitations for TPE(OH)₂(CONH₂)₂ using the TD-LC-DFTB2 and ω B97xD approaches.

Method	State	Excitation energies(eV)	Oscillator Strength	Configuration (coefficient)
TD-LC-DFTB2	1	4.150	0.104	H (106a) $\rightarrow$ L (107a) (0.968)
	2	4.296	0.071	H-2 $\rightarrow$ L (0.827)
	3	4.534	0.014	H-4 $\rightarrow$ L (0.829)
	4	4.555	0.005	H-3 $\rightarrow$ L (0.822)
	5	4.608	0.007	H-1 $\rightarrow$ L (0.665)

	6	4.630	0.043	H-4 $\rightarrow$ L+1 (0.828)
	7	4.717	0.024	H-4 $\rightarrow$ L+1 (0.824)
	8	4.731	0.009	H-3 $\rightarrow$ L (0.828)
	9	4.852	0.001	H-7 $\rightarrow$ L (0.819)
	10	4.948	0.007	H-5 $\rightarrow$ L (0.985)
ω B97xD	1	3.975	0.130	H-1 (147a) $\rightarrow$ L (149a) (0.856)
	2	4.138	0.051	H $\rightarrow$ L (0.826)
	3	4.673	0.025	H-2 $\rightarrow$ L (0.714)
	4	4.775	0.050	H-1 $\rightarrow$ L+1 (0.742)
	5	4.837	0.049	H $\rightarrow$ L+1 (0.457)
	6	4.885	0.004	H-1 $\rightarrow$ L+2 (0.449)
	7	4.989	0.049	H-4 $\rightarrow$ L (0.720)
	8	5.009	0.066	H-1 $\rightarrow$ L+2 (0.544)
	9	5.058	0.026	H-1 $\rightarrow$ L+3 (0.580)
	10	5.101	0.004	H $\rightarrow$ L+1 (0.718)

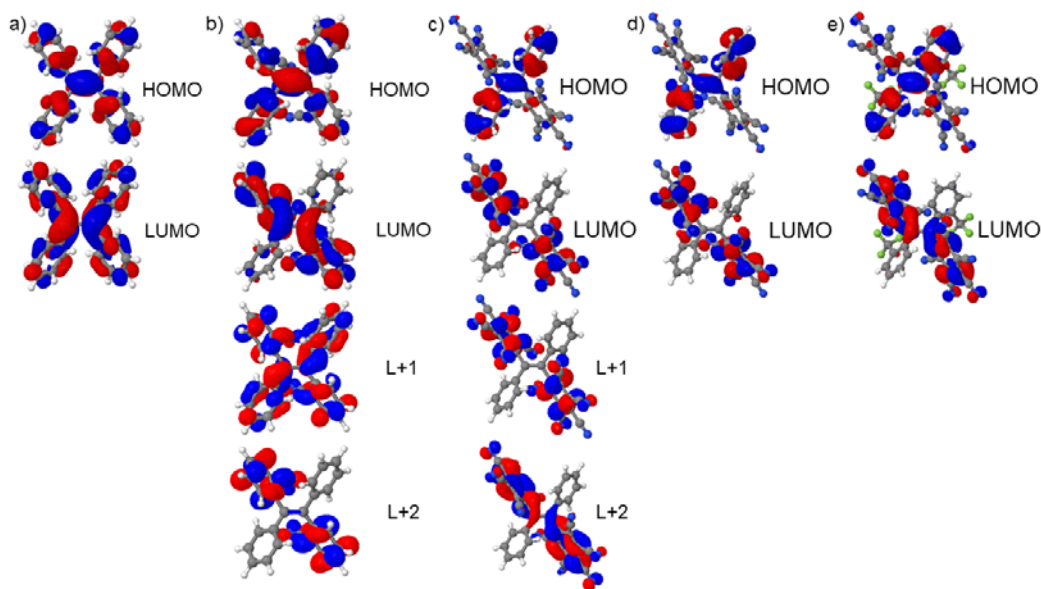


Figure S1. HOMO and LUMO of (a) TPE, (b) TPE(CN), (c) TPE(CN)₅, (d) TPE(CN)₅OH, and (e) TPE(CN)₅CF₃ using the ω B97xD approach.

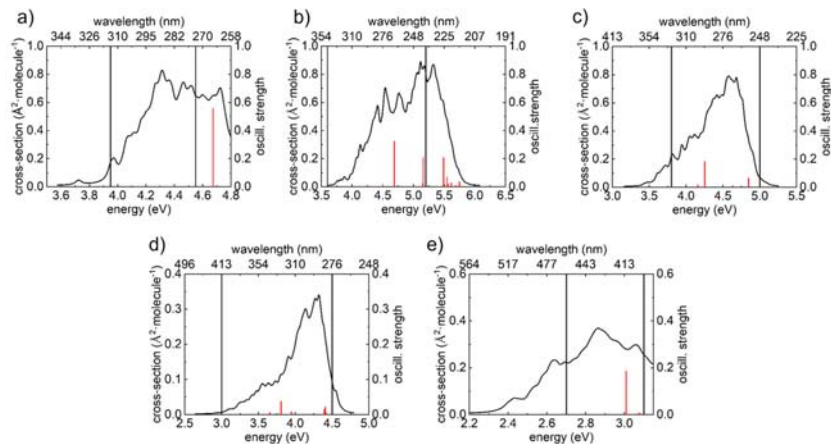


Figure S2. Simulated spectra for group I substituted TPE compounds: a) TPE, b) TPE(CN), c) TPE(CN)₅, d) TPE(CN)₅(OH), e) TPE(CN)₅(CF₃); 250 points and 10 states were calculated with TD-LC-DFTB2. Vertical lines indicate the boundaries of the window for the initial conditions of the dynamics.

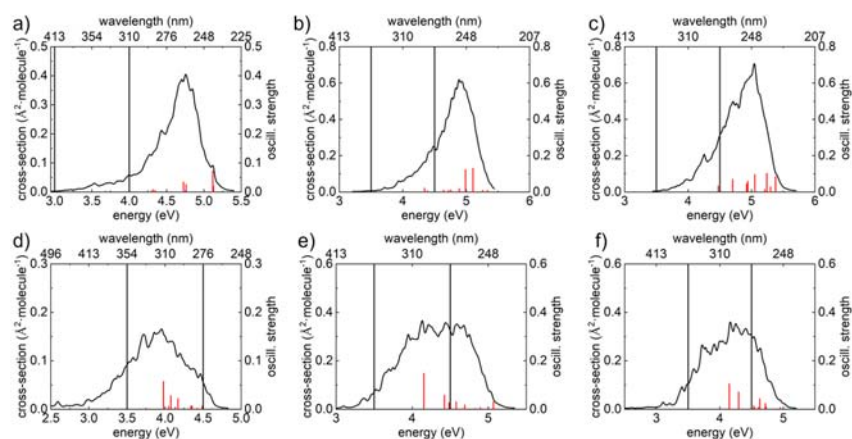


Figure S3. Simulated spectra for group II substituted TPE compounds: a) TPE(OH)(CHO), b) TPE(OH)(COOH), c) TPE(OH)(CONH₂), d) TPE(OH)₂(CHO)₂, e) TPE(OH)₂(COOH)₂, f) TPE(OH)₂(CONH₂)₂; 250 points and 10 states were calculated with TD-LC-DFTB2. Vertical lines indicate the boundaries of the window for the initial conditions of the dynamics.

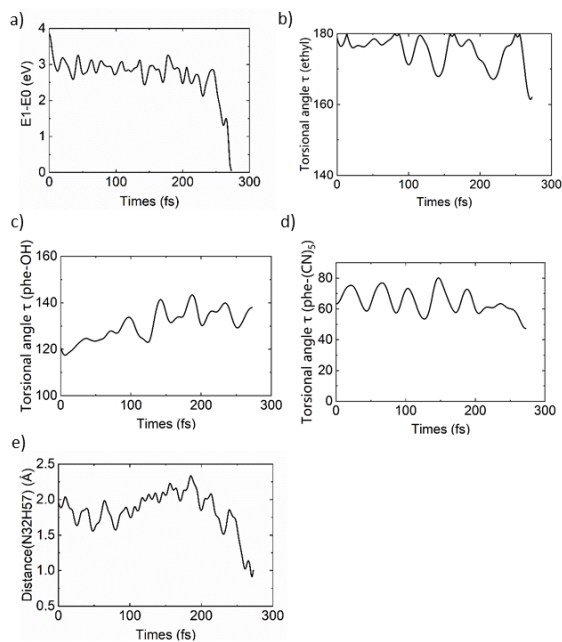


Figure S4. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN)₅(OH) using ω B97XD dynamics simulations.

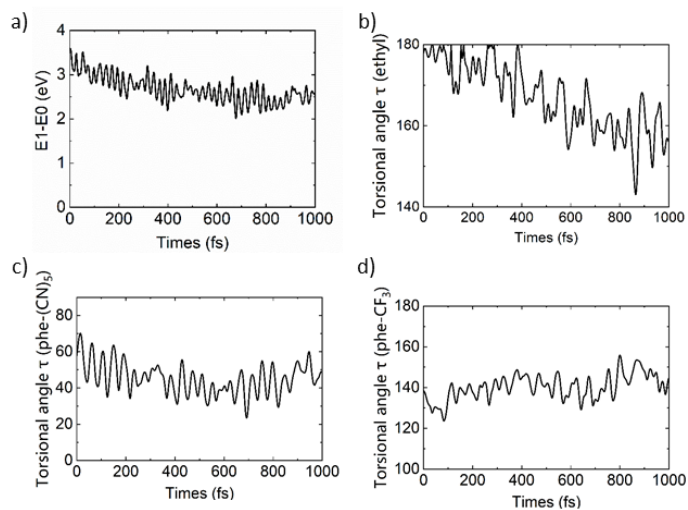


Figure S5. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN)₅(CF₃) using ω B97XD dynamics simulations.

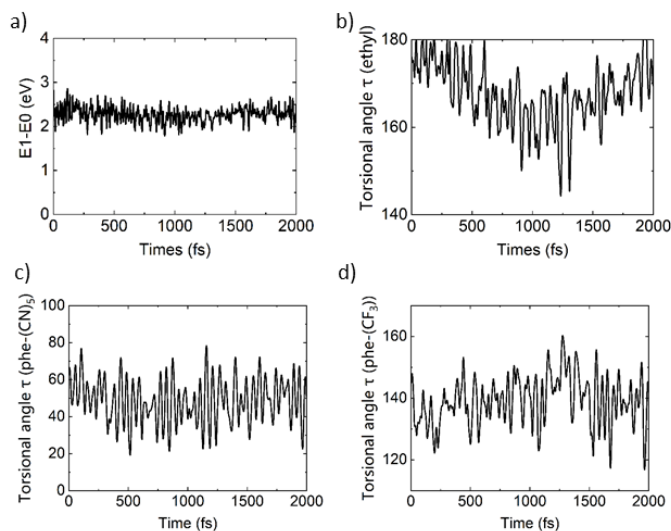


Figure S6. Time evolution of the energy gap $\Delta E(S_1/S_0)$ and the torsional angles τ_{ethyl} and τ_{phenyl} for TPE(CN)₅(CF₃) using LC-DFTB dynamics simulations.

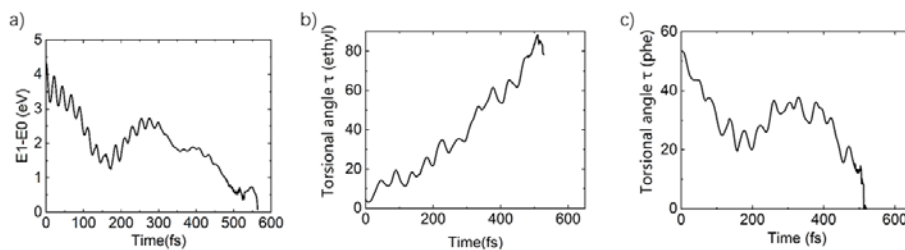


Figure S7. Averaged values for TPE with TD-LC-DFTB2.

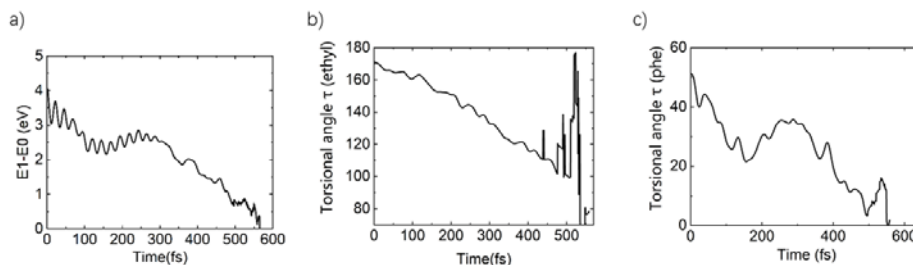


Figure S8. Averaged values for TPE with ω B97XD.

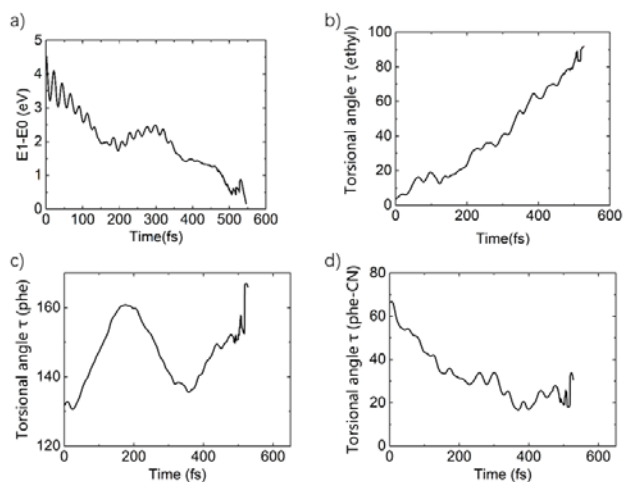


Figure S9. Averaged values for TPE(CN) with TD-LC-DFTB2.

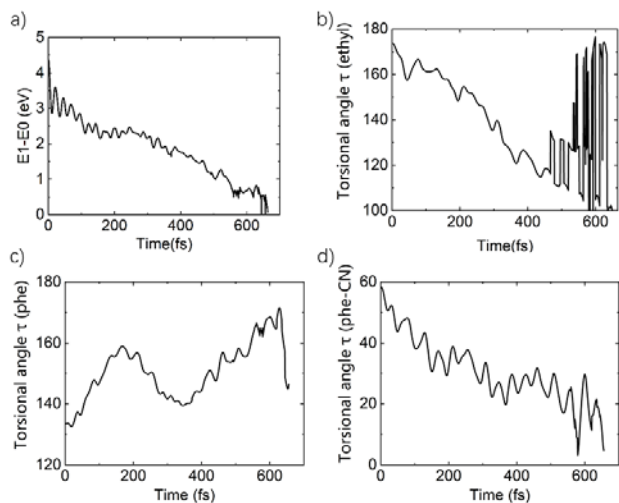


Figure S10. Averaged values for TPE(CN) with ω B97XD.

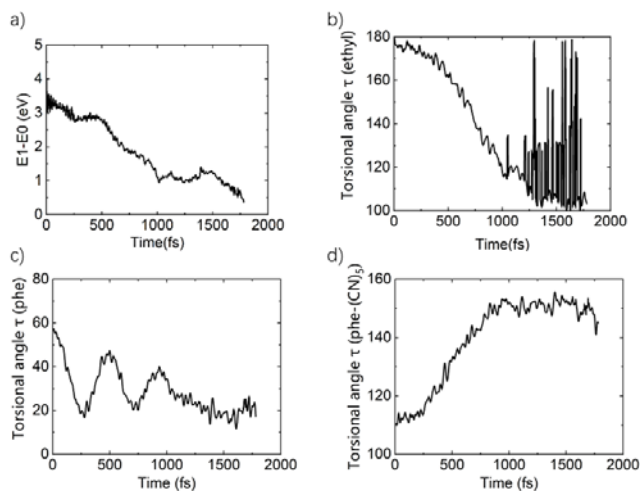


Figure S11. Averaged values for TPE(CN)₅ with TD-LC-DFTB2.

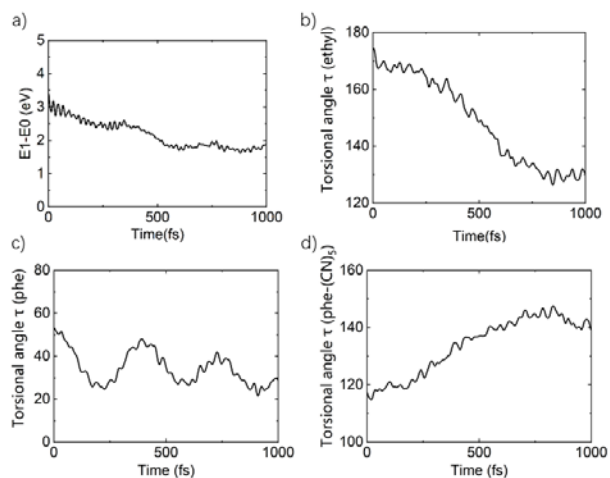


Figure S12. Averaged values for TPE(CN)₅ with ω B97XD.

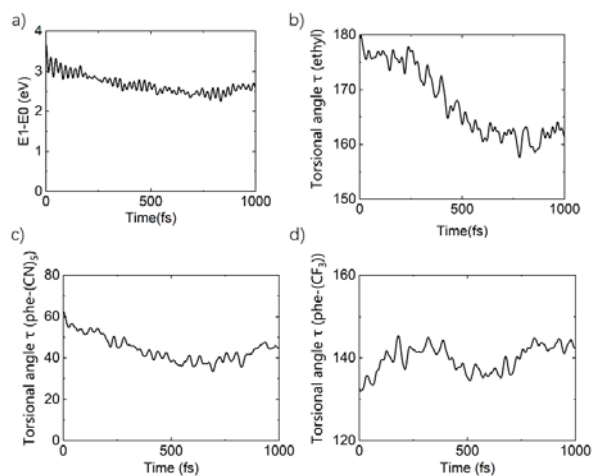


Figure S13. Averaged values for TPE(CN)₅(CF₃) with ω B97XD.

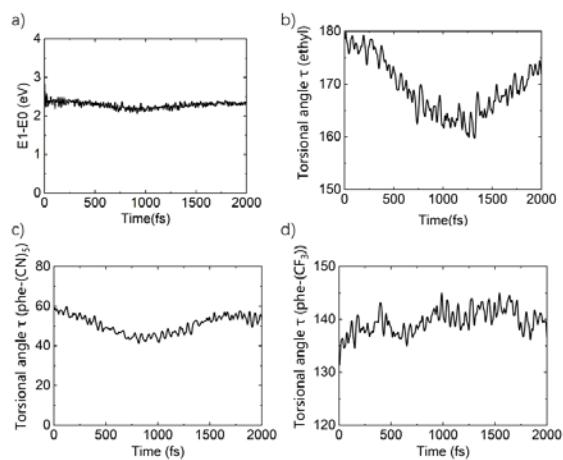


Figure S14. Averaged values for TPE(CN)₅(CF₃) with TD-LC-DFTB2.

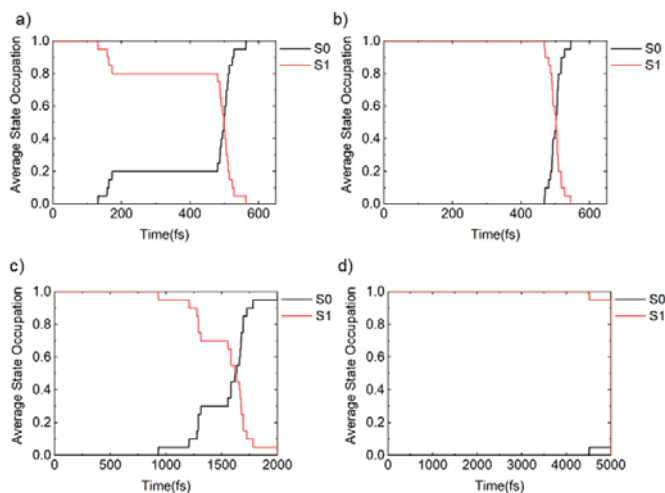


Figure S15. The average occupation for a) TPE, b) TPE(CN), c) TPE(CN)₅, d) TPE(CN)₅OH with TD-LC-DFTB2.

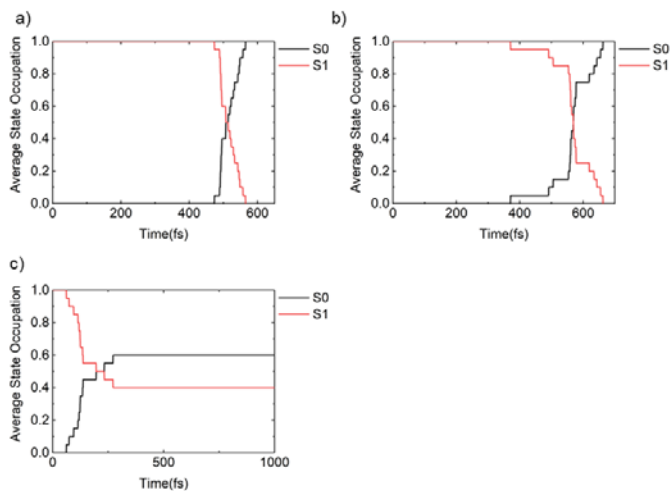


Figure S16. The average occupation for a) TPE, b) TPE(CN), c) TPE(CN)₅OH with ω B97XD.

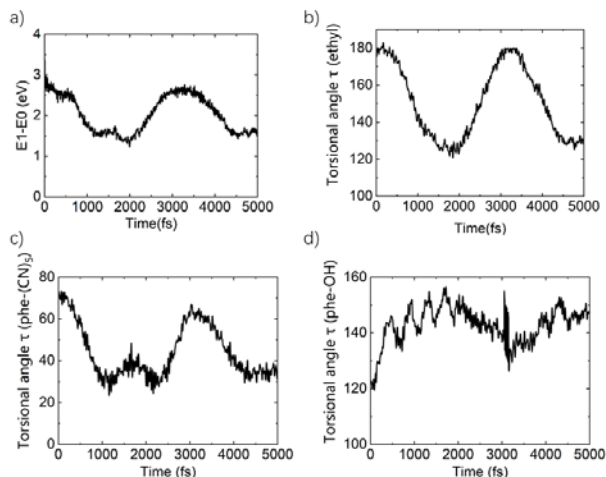


Figure S17. Averaged values for TPE(CN)₅(OH) with TD-LC-DFTB2.

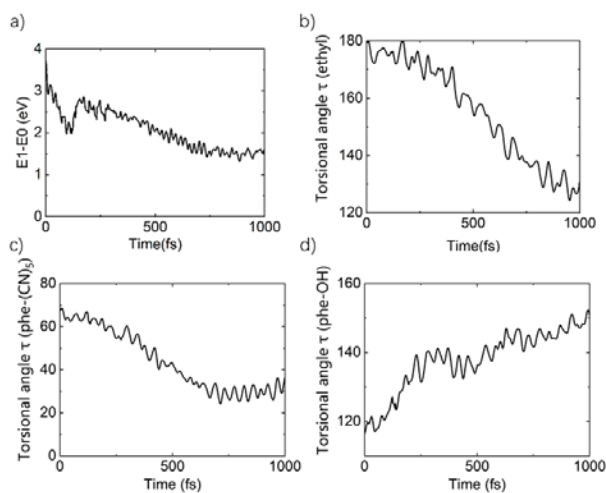


Figure S18. Averaged values for TPE(CN)₅(OH) with ω B97XD.

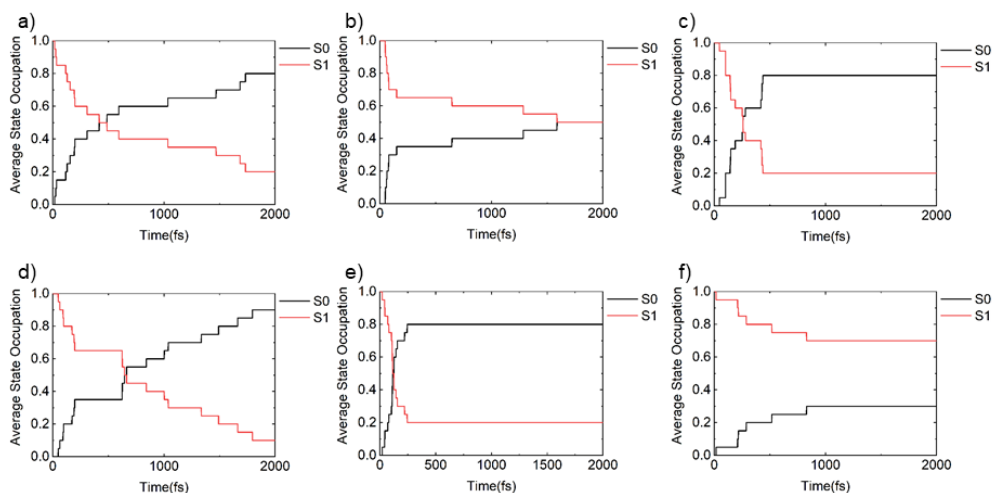


Figure S19. The average occupation for a) TPE(OH)(CHO), b) TPE(OH)₂(CHO)₂, c)

TPE(OH)(CONH₂), d) TPE(OH)₂(CONH₂)₂, e) TPE(OH)(COOH), f)
TPE(OH)₂(COOH)₂ with TD-LC-DFTB2.

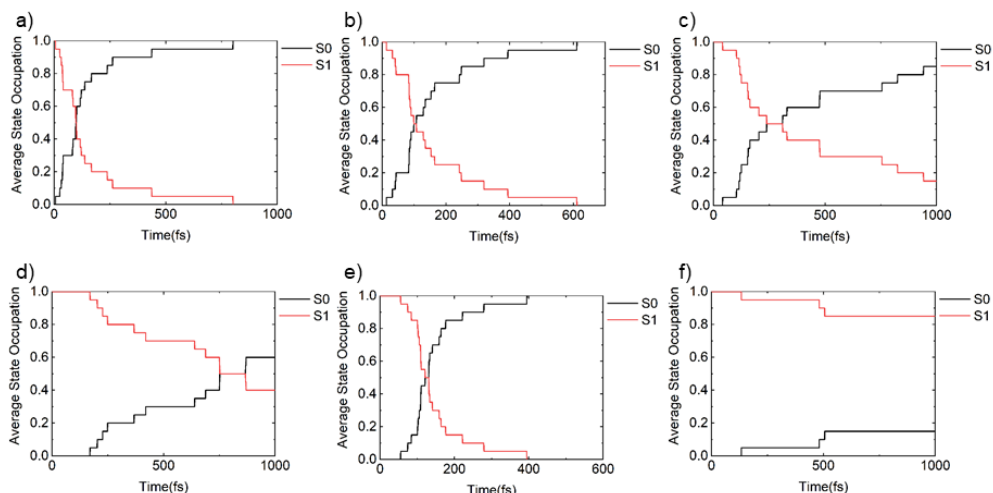


Figure S20. The average occupation for a) TPE(OH)(CHO), b) TPE(OH)₂(CHO)₂, c) TPE(OH)(CONH₂), d) TPE(OH)₂(CONH₂)₂, e) TPE(OH)(COOH), f) TPE(OH)₂(COOH)₂ with ω B97XD.

Cartesian Coordinates (Å) for and total energies (a.u.) for ω B97xD and TD-LC-DFTB2 in S₀ and S₁.

TPE in S₀

ω B97xD, E = -1002.77072 a.u.:

C	-0.00001800	0.67293500	0.00005800
C	-1.25140900	1.47942000	0.06148900
C	0.00001800	-0.67293500	0.00005800
C	1.25133100	1.47948100	-0.06143500
C	1.25140900	-1.47942100	0.06148900
C	-1.25133100	-1.47948100	-0.06143500
C	-1.46656000	2.48840700	-0.87651300
C	-2.62575500	3.24658200	-0.84819800
C	-3.57969500	3.02310500	0.13494400
C	-3.36361100	2.03877000	1.08875800
C	-2.20891400	1.27250400	1.05206200
C	-2.20884000	-1.27254000	-1.05199800
C	-3.36350200	-2.03885600	-1.08875400
C	-3.57954400	-3.02326900	-0.13501100
C	-2.62560000	-3.24676900	0.84812200
C	-1.46644000	-2.48854100	0.87649800
C	2.20884000	1.27253900	-1.05199800

C	3.36350200	2.03885600	-1.08875400
C	3.57954400	3.02326900	-0.13501100
C	2.62559900	3.24676900	0.84812100
C	1.46644000	2.48854100	0.87649800
C	1.46656000	-2.48840700	-0.87651400
C	2.62575600	-3.24658100	-0.84819800
C	3.57969500	-3.02310500	0.13494400
C	3.36361100	-2.03877100	1.08875900
C	2.20891400	-1.27250500	1.05206300
H	-0.71651800	2.67459800	-1.63639300
H	-2.78295300	4.01708000	-1.59321200
H	-4.48489200	3.61731000	0.16128800
H	-4.09868000	1.86434000	1.86495700
H	-2.04888200	0.49815300	1.79200200
H	-2.04884000	-0.49812600	-1.79188000
H	-4.09857600	-1.86440500	-1.86494300
H	-4.48471300	-3.61751400	-0.16140200
H	-2.78276600	-4.01732600	1.59308100
H	-0.71639500	-2.67474800	1.63637000
H	2.04884100	0.49812500	-1.79187900
H	4.09857600	1.86440500	-1.86494200
H	4.48471200	3.61751500	-0.16140200
H	2.78276400	4.01732700	1.59308000
H	0.71639400	2.67474900	1.63636900
H	0.71652000	-2.67459700	-1.63639400
H	2.78295400	-4.01707800	-1.59321300
H	4.48489200	-3.61731000	0.16128800
H	4.09868000	-1.86434200	1.86495800
H	2.04888100	-0.49815500	1.79200300

TD-LC-DFTB2, E = -82.68588 a.u.:

C	-0.012759	0.000044	0.010276
C	-0.071540	0.043209	1.516612
C	1.168896	0.000044	-0.677777
C	-1.351824	-0.043150	-0.682120
C	1.227683	0.043211	-2.184116
C	2.507972	-0.043149	0.014622
C	-0.832273	-0.913665	2.227147
C	-0.899419	-0.876873	3.628209
C	-0.218458	0.122699	4.342736
C	0.528175	1.087536	3.646981
C	0.601484	1.050063	2.246244
C	2.810301	-1.049996	0.960098
C	4.064725	-1.087527	1.587686

C	5.038390	-0.122757	1.281699
C	4.753111	0.876822	0.336793
C	3.501447	0.913672	-0.296314
C	-1.654160	-1.049994	-1.627596
C	-2.908581	-1.087525	-2.255185
C	-3.882252	-0.122756	-1.949203
C	-3.596966	0.876819	-1.004296
C	-2.345304	0.913670	-0.371189
C	1.988416	-0.913664	-2.894647
C	2.055565	-0.876874	-4.295710
C	1.374604	0.122699	-5.010232
C	0.627971	1.087535	-4.314480
C	0.554660	1.050063	-2.913741
H	-1.364384	-1.696163	1.682006
H	-1.484783	-1.627508	4.163005
H	-0.271600	0.151136	5.432576
H	1.054181	1.871393	4.195599
H	1.182080	1.808452	1.717028
H	2.063438	-1.808336	1.203870
H	4.282205	-1.871386	2.315949
H	6.012478	-0.151251	1.773371
H	5.507175	1.627407	0.091634
H	3.289999	1.696177	-1.028165
H	-0.907293	-1.808338	-1.871370
H	-3.126062	-1.871388	-2.983451
H	-4.856330	-0.151251	-2.440871
H	-4.351035	1.627409	-0.759136
H	-2.133856	1.696178	0.360666
H	2.520527	-1.696163	-2.349505
H	2.640928	-1.627506	-4.830504
H	1.427747	0.151137	-6.100078
H	0.101964	1.871395	-4.863100
H	-0.025936	1.808451	-2.384530

TPE in S_1

ω B97xD, not converged:

TD-LC-DFTB2, not converged:

TPE(CN)₂ in S_0

ω B97xD, E = -1187.24191 a.u.:

C	-1.32442600	-2.58553600	0.54824100
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C	-1.16493300	-1.55110500	-0.37241100
C	-2.12230100	-1.38514000	-1.37091500
C	-3.22553200	-2.22300600	-1.43480200
C	-3.38531200	-3.23612000	-0.50101700
C	-2.43091900	-3.41488100	0.49099300
C	0.03257700	-0.67127900	-0.28917300
C	1.32742500	-1.40586800	-0.24580700
C	2.24498900	-1.27847500	0.80498400
C	3.44697500	-1.98892500	0.78708800
C	3.74139200	-2.83384700	-0.26553700
C	2.82595900	-2.98840300	-1.29847900
C	1.63198300	-2.29075900	-1.27806700
C	1.97934900	-0.44152500	1.93784500
N	1.81475300	0.21042200	2.87013100
H	4.14036400	-1.87120500	1.60953400
H	4.67659200	-3.37856700	-0.27517300
H	3.04339500	-3.65935100	-2.12021200
H	0.91276000	-2.42155300	-2.07749500
C	-0.03258400	0.67126900	-0.28917600
C	-1.32743100	1.40585900	-0.24581400
C	-2.24498200	1.27849900	0.80499400
C	-3.44696700	1.98895200	0.78709300
C	-3.74139300	2.83384700	-0.26555100
C	-2.82597300	2.98837200	-1.29850900
C	-1.63199900	2.29072500	-1.27809300
C	-1.97932800	0.44159300	1.93788400
N	-1.81471300	-0.21035900	2.87016300
H	-4.14034400	1.87126000	1.60955200
H	-4.67659100	3.37857100	-0.27518900
H	-3.04341600	3.65929900	-2.12025700
H	-0.91278400	2.42149600	-2.07753200
C	1.16492600	1.55109300	-0.37242300
C	2.12228300	1.38513200	-1.37093900
C	3.22551500	2.22299500	-1.43483300
C	3.38530900	3.23610300	-0.50104400
C	2.43092800	3.41485900	0.49097800
C	1.32443200	2.58551800	0.54823300
H	0.58951500	2.71848600	1.33266800
H	2.55182300	4.19876600	1.22802800
H	4.24996700	3.88674600	-0.54670500
H	3.96167400	2.08328300	-2.21695300
H	2.00118800	0.59525800	-2.10196400
H	-0.58950000	-2.71850700	1.33266700
H	-2.55180400	-4.19879200	1.22803900

H	-4.24996900	-3.88676500	-0.54667200
H	-3.96170100	-2.08329100	-2.21691200
H	-2.00121600	-0.59526100	-2.10193600

TD-LC-DFTB2, E = -72.00828 a.u.:

C	1.068829	2.379132	-1.058972
C	0.109432	1.954838	-0.111084
C	-0.365973	2.889097	0.837366
C	0.094262	4.214991	0.826513
C	1.035779	4.628601	-0.129634
C	1.521707	3.706395	-1.071446
C	-0.370733	0.525100	-0.107571
C	0.730695	-0.509636	-0.110321
C	0.904734	-1.422148	-1.188429
C	1.960855	-2.362123	-1.149365
C	2.842191	-2.401223	-0.060644
C	2.683672	-1.491104	0.998153
C	1.642732	-0.551751	0.967732
C	0.027633	-1.406569	-2.334807
N	-0.659788	-1.424288	-3.268271
H	2.086853	-3.060777	-1.977914
H	3.651018	-3.133457	-0.038977
H	3.371212	-1.512534	1.845649
H	1.526485	0.150993	1.795145
C	-1.694848	0.189998	-0.085082
C	-2.796688	1.223574	-0.123902
C	-2.992489	2.074518	-1.247659
C	-4.048156	3.015783	-1.240326
C	-4.907848	3.116129	-0.138306
C	-4.727946	2.266504	0.966351
C	-3.687285	1.326353	0.967911
C	-2.138202	1.994452	-2.408483
N	-1.469392	1.959655	-3.354903
H	-4.190878	3.667123	-2.103967
H	-5.716502	3.848870	-0.141618
H	-5.398634	2.335621	1.824737
H	-3.554329	0.670869	1.830842
C	-2.174207	-1.237437	0.000814
C	-1.679659	-2.117512	0.990404
C	-2.139273	-3.441693	1.062710
C	-3.099240	-3.907554	0.149925
C	-3.604195	-3.039127	-0.832139
C	-3.151906	-1.713488	-0.902755
H	-3.543302	-1.049402	-1.675877

H	-4.350494	-3.395690	-1.544644
H	-3.452306	-4.938985	0.204533
H	-1.746669	-4.109205	1.832419
H	-0.938826	-1.765963	1.711714
H	1.445236	1.672692	-1.801380
H	2.253594	4.022191	-1.817349
H	1.389311	5.661266	-0.139684
H	-0.283438	4.924669	1.565335
H	-1.092239	2.578799	1.591657

TPE(CN)₂ in S₁

ωB97xD, E = -1187.13150 a.u.:

C	1.15763800	2.85821500	-0.54752200
C	0.87443500	1.52341600	-0.89997900
C	1.62253800	0.94929000	-1.94591800
C	2.55944100	1.68850000	-2.64190400
C	2.80324800	3.01126700	-2.29693800
C	2.10634500	3.58479100	-1.23824000
C	-0.09680300	0.72420800	-0.18118500
C	-1.28068200	1.28245800	0.40533800
C	-1.99878900	0.62926200	1.44585700
C	-3.18756000	1.16374500	1.94349900
C	-3.70704600	2.33203700	1.42571600
C	-3.03277300	2.97898200	0.39029400
C	-1.85363600	2.47200200	-0.10238400
C	-1.51462100	-0.55519200	2.07748000
N	-1.18947700	-1.50256800	2.64781600
H	-3.69295600	0.64773200	2.74963100
H	-4.63260400	2.73468600	1.81577600
H	-3.44539400	3.88235300	-0.04176800
H	-1.37101100	2.96604700	-0.93409200
C	0.09554900	-0.72477500	-0.18059400
C	1.27975600	-1.28238500	0.40589600
C	2.00077700	-0.62625800	1.44261400
C	3.18955500	-1.16072900	1.94014900
C	3.70627200	-2.33179800	1.42585000
C	3.02918700	-2.98159400	0.39405100
C	1.84996000	-2.47465500	-0.09843300
C	1.52020400	0.56192700	2.07001500
N	1.19730200	1.51252200	2.63638700
H	3.69728500	-0.64236800	2.74330400
H	4.63191400	-2.73438500	1.81576500
H	3.43964300	-3.88721700	-0.03535600

H	1.36496500	-2.97110400	-0.92736100
C	-0.87566600	-1.52484800	-0.89817700
C	-1.62604600	-0.95139200	-1.94288900
C	-2.56285600	-1.69167300	-2.63787800
C	-2.80421800	-3.01494800	-2.29315900
C	-2.10488800	-3.58793500	-1.23572900
C	-1.15629900	-2.86027700	-0.54602100
H	-0.66312400	-3.29354500	0.31411000
H	-2.31632100	-4.60712500	-0.93644900
H	-3.54696200	-3.59155900	-2.83037500
H	-3.11173000	-1.23307100	-3.45116000
H	-1.44495100	0.08141600	-2.21539900
H	0.66638800	3.29178700	0.31353700
H	2.31976200	4.60350700	-0.93875100
H	3.54609100	3.58701000	-2.83494900
H	3.10649500	1.22946700	-3.45616800
H	1.43959700	-0.08315200	-2.21858200

TD-LC-DFTB2, E = -71.94039 a.u.:

C	1.0742739	2.9106247	-0.7719586
C	0.8088003	1.5287338	-1.0082961
C	1.5344730	0.8918691	-2.0590645
C	2.4323826	1.6068637	-2.8595568
C	2.6562456	2.9748412	-2.6257737
C	1.9811488	3.6154958	-1.5705729
C	-0.1036064	0.7386262	-0.1614411
C	-1.2581341	1.3027185	0.5283413
C	-1.9692490	0.5601023	1.5382624
C	-3.1198176	1.1106874	2.1504265
C	-3.5986205	2.3730804	1.7833240
C	-2.9280846	3.1041152	0.7796886
C	-1.7886634	2.5831836	0.1693580
C	-1.5452583	-0.7376306	1.9916455
N	-1.3022521	-1.7744126	2.4616142
H	-3.6373640	0.5355245	2.9198942
H	-4.4884502	2.7839154	2.2625494
H	-3.3085328	4.0800658	0.4718828
H	-1.3040995	3.1543773	-0.6264824
C	0.1030043	-0.7394218	-0.1603890
C	1.2581641	-1.3024622	0.5292418
C	1.9702397	-0.5585657	1.5375788
C	3.1214305	-1.1082657	2.1492782
C	3.6001074	-2.3710415	1.7832477
C	2.9285038	-3.1034704	0.7813524

C	1.7883968	-2.5834600	0.1715875
C	1.5468473	0.7397543	1.9898622
N	1.3047271	1.7772098	2.4588763
H	3.6396486	-0.5321328	2.9175755
H	4.4905595	-2.7810817	2.2619569
H	3.3086621	-4.0798320	0.4744718
H	1.3029182	-3.1558377	-0.6228502
C	-0.8101651	-1.5306214	-1.0054758
C	-1.5369675	-0.8950603	-2.0562567
C	-2.4353674	-1.6109292	-2.8551671
C	-2.6588646	-2.9787008	-2.6198690
C	-1.9826943	-3.6181781	-1.5646000
C	-1.0752813	-2.9123504	-0.7674616
H	-0.6051120	-3.4196415	0.0774929
H	-2.1751944	-4.6724607	-1.3557055
H	-3.3632946	-3.5362732	-3.2394871
H	-2.9674400	-1.1009695	-3.6608761
H	-1.3740160	0.1685791	-2.2495935
H	0.6048233	3.4188231	0.0728412
H	2.1741050	4.6699160	-1.3628122
H	3.3601902	3.5316616	-3.2466334
H	2.9636927	1.0959532	-3.6650919
H	1.3711191	-0.1718480	-2.2512099

TPE (CN)₅ in S₀

ωB97xD, E = -1925.04167 a.u.:

C	0.99348600	2.36818200	-1.04562400
C	0.09371300	1.94025800	-0.07125300
C	-0.34370100	2.84172900	0.89777600
C	0.14038700	4.13867000	0.91392800
C	1.05180700	4.55211800	-0.04712300
C	1.47200100	3.66768200	-1.03046200
C	-0.39950700	0.53871600	-0.03958700
C	-1.88270900	0.39113500	0.00169600
C	-2.54849500	-0.11750400	1.12077200
C	-3.94736300	-0.20026500	1.14927900
C	-4.69928300	0.22477800	0.05196800
C	-4.04426800	0.72817800	-1.07577500
C	-2.64898900	0.80944400	-1.09259900
C	-1.81989600	-0.57943100	2.26174300
C	-4.60987800	-0.72637500	2.30166300
C	-6.12561900	0.14072200	0.07852400
C	-4.80137900	1.14762900	-2.21350300

C	-1.99146400	1.26828800	-2.27812600
C	0.39948600	-0.53876100	-0.03952100
C	1.88268200	-0.39113800	0.00175300
C	2.54846200	0.11762200	1.12077600
C	3.94732900	0.20042400	1.14926200
C	4.69924900	-0.22469900	0.05198100
C	4.04423700	-0.72821600	-1.07571200
C	2.64896000	-0.80952000	-1.09251300
C	1.81986100	0.57961700	2.26171900
C	4.60984200	0.72663800	2.30159900
C	6.12558400	-0.14060900	0.07851900
C	4.80134700	-1.14776300	-2.21340400
C	1.99142400	-1.26851400	-2.27797600
C	-0.09368900	-1.94032200	-0.07109200
C	-0.99330100	-2.36840500	-1.04554100
C	-1.47175700	-3.66792500	-1.03029900
C	-1.05166100	-4.55222800	-0.04679800
C	-0.14039200	-4.13862800	0.91433000
C	0.34364100	-2.84166800	0.89809400
H	-1.03415900	2.51816500	1.66773400
H	-0.18921600	4.82564000	1.68247600
H	1.42945800	5.56665900	-0.03461900
H	2.16265300	3.99404100	-1.79738700
H	1.28667900	1.69338200	-1.84017800
H	1.03398200	-2.51798700	1.66810700
H	0.18913800	-4.82549500	1.68300100
H	-1.42926400	-5.56678600	-0.03423300
H	-2.16227900	-3.99440800	-1.79728700
H	-1.28640400	-1.69371900	-1.84022500
N	1.27318400	0.97921700	3.18886200
N	5.14430500	1.15056900	3.22522100
N	7.27165200	-0.07318600	0.09828000
N	5.40768700	-1.48571200	-3.12807400
N	1.45981700	-1.60387900	-3.23907900
N	-1.45989100	1.60354200	-3.23928700
N	-5.40771800	1.48550200	-3.12820200
N	-7.27169000	0.07332700	0.09830000
N	-5.14434500	-1.15021300	3.22532500
N	-1.27321200	-0.97897300	3.18890700

TD-LC-DFTB2, E = -107.69731 a.u.:

C	1.0072361	2.4238065	-0.9902345
C	0.1052333	1.9618489	-0.0050592

C	-0.3063919	2.8497172	1.0147912
C	0.1900945	4.1610646	1.0590166
C	1.0909898	4.6088428	0.0790854
C	1.4929596	3.7396935	-0.9478069
C	-0.4130052	0.5424008	-0.0173063
C	-1.9193962	0.4011000	-0.0190662
C	-2.6222542	-0.0783626	1.1180968
C	-4.0404090	-0.1861065	1.0932637
C	-4.7653873	0.1930419	-0.0670135
C	-4.0670733	0.6792828	-1.2042932
C	-2.6501769	0.7821744	-1.1767969
C	-1.9151457	-0.4714613	2.3136657
C	-4.7414781	-0.6868669	2.2499221
C	-6.2033020	0.0824484	-0.0921660
C	-4.7937258	1.0679815	-2.3878380
C	-1.9502657	1.2480894	-2.3503438
C	0.4130291	-0.5424332	-0.0177081
C	1.9194204	-0.4010898	-0.0193932
C	2.6222791	0.0776468	1.1180761
C	4.0404338	0.1854218	1.0933102
C	4.7654167	-0.1930128	-0.0671973
C	4.0671000	-0.6784718	-1.2048088
C	2.6501996	-0.7813497	-1.1773930
C	1.9151769	0.4699038	2.3139268
C	4.7414876	0.6855052	2.2502713
C	6.2033328	-0.0824180	-0.0922673
C	4.7937522	-1.0663075	-2.3886375
C	1.9502876	-1.2463665	-2.3512957
C	-0.1052107	-1.9619093	-0.0064849
C	-1.0071629	-2.4231472	-0.9920201
C	-1.4929022	-3.7391065	-0.9505390
C	-1.0909669	-4.6089506	0.0757426
C	-0.1901299	-4.1618981	1.0560245
C	0.3063786	-2.8504773	1.0127463
H	-0.9972222	2.5061195	1.7873166
H	-0.1265019	4.8319039	1.8593721
H	1.4743041	5.6298963	0.1133291
H	2.1832119	4.0854785	-1.7192289
H	1.3127048	1.7622684	-1.8033075
H	0.9971810	-2.5074686	1.7855437
H	0.1264478	-4.8332855	1.8559163
H	-1.4742817	-5.6300514	0.1092341
H	-2.1831104	-4.0843163	-1.7222459
H	-1.3126140	-1.7610754	-1.8046512

N	1.3596728	0.8001263	3.2753262
N	5.3042329	1.0913269	3.1779940
N	7.3580263	0.0073905	-0.1133831
N	5.3766629	-1.3816342	-3.3387806
N	1.3831006	-1.6063741	-3.2951857
N	-1.3830679	1.6088567	-3.2939374
N	-5.3766269	1.3840668	-3.3377354
N	-7.3579984	-0.0073103	-0.1133476
N	-5.3042601	-1.0932050	3.1773968
N	-1.3596425	-0.8024453	3.2748050

TPE(CN)₅ in S₁

ω B97xD, E = -1924.93830 a.u.:

C	-0.99555800	-1.93109100	-1.86649400
C	-0.00594800	-1.84960900	-0.86474700
C	0.51646500	-3.04731300	-0.33612600
C	0.07980800	-4.26636100	-0.80241500
C	-0.87909400	-4.32523100	-1.80952400
C	-1.41304800	-3.15524500	-2.34064300
C	0.45146800	-0.56440900	-0.39549800
C	1.80317700	-0.37280800	0.06288300
C	2.11648800	0.50018500	1.14697500
C	3.43723900	0.71804200	1.54349900
C	4.49897300	0.09409400	0.88247500
C	4.21894600	-0.73393000	-0.21786100
C	2.90755200	-0.95208600	-0.62608200
C	1.09206000	1.13617400	1.90947900
C	3.71361900	1.59103200	2.64333400
C	5.84388600	0.31857200	1.29446100
C	5.29928300	-1.33028600	-0.94110500
C	2.70799000	-1.65116100	-1.85790600
C	-0.45146600	0.56442600	-0.39546900
C	-1.80315700	0.37284500	0.06295100
C	-2.11645500	-0.50013100	1.14706400
C	-3.43721400	-0.71807000	1.54357800
C	-4.49897000	-0.09421500	0.88252000
C	-4.21894900	0.73388400	-0.21777800
C	-2.90756900	0.95214900	-0.62598700
C	-1.09200400	-1.13599500	1.90963600
C	-3.71354900	-1.59109300	2.64338100
C	-5.84387200	-0.31883200	1.29442100
C	-5.29930600	1.33021000	-0.94102400
C	-2.70807600	1.65129100	-1.85777800

C	0.00599200	1.84962700	-0.86469600
C	0.99554700	1.93115500	-1.86651000
C	1.41299700	3.15532100	-2.34063600
C	0.87903400	4.32529100	-1.80946200
C	-0.07984500	4.26637400	-0.80234400
C	-0.51644700	3.04729800	-0.33605900
H	1.22621200	-3.00123300	0.48001900
H	0.47479100	-5.17854200	-0.37519800
H	-1.21788800	-5.28603100	-2.17618200
H	-2.15269200	-3.20450500	-3.12892300
H	-1.38997400	-1.02181100	-2.30386300
H	-1.22617900	3.00116100	0.48010200
H	-0.47488300	5.17853900	-0.37514300
H	1.21779900	5.28611300	-2.17608800
H	2.15258800	3.20461200	-3.12896500
H	1.38990800	1.02188600	-2.30395600
N	-0.28512900	-1.66771600	2.53419500
N	-3.93869200	-2.30033300	3.51785500
N	-6.92985000	-0.50017200	1.62441600
N	-6.16846100	1.81168900	-1.51688500
N	-2.57779700	2.15969500	-2.88050300
N	2.57759700	-2.15961300	-2.88059400
N	6.16842700	-1.81175300	-1.51698700
N	6.92985900	0.49977900	1.62454200
N	3.93880700	2.30026000	3.51780400
N	0.28528500	1.66805000	2.53402900

TD-LC-DFTB2, E = -107.69731 a.u.:

C	0.9623202	1.6706466	-1.9504916
C	0.0259026	1.7907027	-0.8835238
C	-0.3591685	3.1009665	-0.4720219
C	0.1647956	4.2295589	-1.1100350
C	1.0710556	4.0893938	-2.1768330
C	1.4671407	2.8064225	-2.5933803
C	-0.4506258	0.5856961	-0.1758352
C	-1.7857337	0.4839368	0.3935615
C	-2.0555998	-0.4140696	1.4929206
C	-3.3528762	-0.5099861	2.0570911
C	-4.4253227	0.2641464	1.5380999
C	-4.1946533	1.1051825	0.4099597
C	-2.9057320	1.2087310	-0.1632367
C	-1.0122797	-1.2068444	2.0869188
C	-3.5847287	-1.4022370	3.1669856
C	-5.7370312	0.1785349	2.1243545

C	-5.2941317	1.8412167	-0.1655342
C	-2.7904651	1.9470647	-1.3978394
C	0.4493278	-0.5912999	-0.1737434
C	1.7854688	-0.4866303	0.3926439
C	2.0576825	0.4183874	1.4857666
C	3.3571510	0.5214815	2.0437339
C	4.4294996	-0.2527781	1.5248817
C	4.1956589	-1.1031144	0.4043701
C	2.9046021	-1.2139728	-0.1626935
C	1.0152094	1.2124415	2.0795468
C	3.5916938	1.4217188	3.1465521
C	5.7444165	-0.1570378	2.1023930
C	5.2945741	-1.8406344	-0.1702163
C	2.7868939	-1.9626581	-1.3907774
C	-0.0284693	-1.7981180	-0.8775938
C	-0.9634644	-1.6785702	-1.9458431
C	-1.4693324	-2.8146444	-2.5874223
C	-1.0760831	-4.0973326	-2.1676210
C	-0.1714826	-4.2369883	-1.0994376
C	0.3539200	-3.1080561	-0.4628490
H	-1.0319336	3.2276110	0.3791475
H	-0.1301670	5.2244419	-0.7720629
H	1.4700963	4.9742664	-2.6753613
H	2.1711464	2.6920547	-3.4194826
H	1.2659661	0.6759339	-2.2867744
H	1.0258946	-3.2345967	0.3889250
H	0.1214386	-5.2318966	-0.7596188
H	-1.4760904	-4.9824290	-2.6650303
H	-2.1714607	-2.7005191	-3.4149999
H	-1.2648333	-0.6839530	-2.2845084
N	0.2231442	1.8731512	2.6158822
N	3.7852928	2.1501573	4.0263990
N	6.8034948	-0.0794870	2.5675852
N	6.1790575	-2.4337547	-0.6264810
N	2.7971293	-2.5010487	-2.4191454
N	-2.8012999	2.4761992	-2.4309701
N	-6.1786140	2.4334341	-0.6229870
N	-6.7931954	0.1106292	2.5976014
N	-3.7754047	-2.1247575	4.0523432
N	-0.2191517	-1.8661916	2.6233870

TPE(CN)₅OH in S₀

ω B97xD, E = -2075.50960 a.u.:

C	0.23394400	2.80660100	-0.89562400
C	-0.10098100	1.93497400	0.14391800
C	-0.91971700	2.39244200	1.17589300
C	-1.40787200	3.68657600	1.16564100
C	-1.07266600	4.54154400	0.12398900
C	-0.24890800	4.10595000	-0.90093300
C	0.40129300	0.53653200	0.11123200
C	1.88603800	0.38180100	0.09376800
C	2.56901300	-0.13103200	-1.01299400
C	3.96326100	-0.22555000	-1.02579000
C	4.70400200	0.19369900	0.08287700
C	4.03556400	0.69276800	1.20230400
C	2.63821800	0.78057900	1.20180900
C	1.84420600	-0.58922000	-2.15745500
N	1.27468600	-1.00028800	-3.06520100
C	4.63371800	-0.75564500	-2.17184000
N	5.16735100	-1.18623100	-3.09285900
C	6.12991600	0.10197600	0.07398100
N	7.27564300	0.02663400	0.06691000
C	4.77855700	1.10068000	2.35346100
N	5.37387300	1.42876400	3.27890400
C	1.97221200	1.22635800	2.38753800
N	1.43848000	1.54763600	3.35226400
C	-0.40121600	-0.53653200	0.11119700
C	-1.88596400	-0.38178500	0.09374600
C	-2.56895800	0.13103200	-1.01301100
C	-3.96320700	0.22556400	-1.02577300
C	-4.70392300	-0.19365300	0.08292100
C	-4.03546300	-0.69270500	1.20234400
C	-2.63811900	-0.78052500	1.20181700
C	-1.84419200	0.58918500	-2.15751400
N	-1.27471000	1.00021100	-3.06530200
C	-4.63368600	0.75564900	-2.17181400
N	-5.16733800	1.18623600	-3.09282200
C	-6.12983600	-0.10191700	0.07405700
N	-7.27556300	-0.02656000	0.06701100
C	-4.77843500	-1.10058700	2.35352500
N	-5.37374000	-1.42864200	3.27898600
C	-1.97208800	-1.22629000	2.38753800
N	-1.43830900	-1.54750600	3.35225800
C	0.10099900	-1.93499400	0.14386600
C	0.91971100	-2.39250300	1.17584400
C	1.40767400	-3.68670900	1.16567800
C	1.07228600	-4.54171900	0.12411900

C	0.24856400	-4.10608000	-0.90081100
C	-0.23407200	-2.80665100	-0.89560800
O	-1.05709100	-2.36647400	-1.90140500
H	-0.02600400	-4.76065300	-1.71801000
H	1.44982500	-5.55634500	0.11306800
H	2.03528500	-4.03227500	1.97650700
H	1.14628600	-1.73401900	2.00516000
O	1.05700100	2.36641500	-1.90138200
H	0.02553000	4.76050800	-1.71818800
H	-1.45038000	5.55610300	0.11285500
H	-2.03550300	4.03211600	1.97646500
H	-1.14617900	1.73398200	2.00526000
H	0.51748800	2.09713500	-2.65770900
H	-0.51750700	-2.09674500	-2.65752900

TD-LC-DFTB2, E = -115.49151 a.u.:

C	-0.1446436	-2.8872522	-1.0318146
C	0.1317506	-1.9640284	0.0115562
C	0.9319031	-2.3998665	1.0963245
C	1.4355541	-3.7066429	1.1479828
C	1.1448778	-4.6099896	0.1088612
C	0.3580745	-4.2029246	-0.9752089
C	-0.4086059	-0.5464533	-0.0180494
C	-1.9176631	-0.3943118	0.0327224
C	-2.6543808	0.0423926	-1.1000379
C	-4.0675882	0.1872607	-1.0349770
C	-4.7560539	-0.1056451	0.1710714
C	-4.0255969	-0.5438968	1.3073963
C	-2.6133659	-0.6891679	1.2363609
C	-1.9759669	0.3420648	-2.3398696
N	-1.4427761	0.6050428	-3.3349395
C	-4.7972709	0.6341504	-2.1957526
N	-5.3827079	0.9934816	-3.1284924
C	-6.1888238	0.0440932	0.2434636
N	-7.3393248	0.1648781	0.3021655
C	-4.7161301	-0.8363968	2.5394086
N	-5.2713903	-1.0711123	3.5285996
C	-1.8939911	-1.1004369	2.4185074
N	-1.3246500	-1.4139258	3.3774579
C	0.4084018	0.5466487	-0.0165590
C	1.9174585	0.3945122	0.0335989
C	2.6539108	-0.0390335	-1.1005203
C	4.0670880	-0.1843691	-1.0361525
C	4.7558816	0.1051057	0.1705188

C	4.0257427	0.5404930	1.3081557
C	2.6134749	0.6860813	1.2378698
C	1.9751998	-0.3350325	-2.3410626
N	1.4417790	-0.5950631	-3.3368101
C	4.7961564	-0.6283760	-2.1984083
N	5.3807402	-0.9855631	-3.1325018
C	6.1886247	-0.0450106	0.2420695
N	7.3391483	-0.1660437	0.2998709
C	4.7166293	0.8299989	2.5406894
N	5.2722241	1.0625732	3.5302152
C	1.8944821	1.0943982	2.4213089
N	1.3255091	1.4056087	3.3812202
C	-0.1320822	1.9641459	0.0166686
C	-0.9318470	2.3972550	1.1028002
C	-1.4358544	3.7038007	1.1576107
C	-1.1453752	4.6097070	0.1206874
C	-0.3587873	4.2054276	-0.9645382
C	0.1437580	2.8898408	-1.0246557
O	0.8833238	2.5455023	-2.1158074
H	-0.1322234	4.8966003	-1.7764572
H	-1.5340663	5.6286404	0.1615858
H	-2.0438219	4.0153228	2.0074763
H	-1.1407307	1.7082451	1.9233307
O	-0.8848789	-2.5403315	-2.1217376
H	0.1315876	-4.8920338	-1.7889066
H	1.5336290	-5.6289868	0.1471117
H	2.0434717	-4.0204126	1.9971122
H	1.1414593	-1.7127583	1.9183067
H	-1.0637188	-1.5783032	-2.1647843
H	1.0624683	1.5836205	-2.1610116

TPE (CN)₅OH in S₁

ω B97xD, E = -2075.41044 a.u.:

C	-0.52823600	-3.08309400	0.35170200
C	-0.03176900	-1.83946000	0.84398500
C	0.87980100	-1.88174800	1.92881800
C	1.20733700	-3.05693900	2.54501300
C	0.65396100	-4.25979200	2.08003600
C	-0.19294800	-4.27114200	0.99810800
C	-0.46532900	-0.55410600	0.35730700
C	-1.82256100	-0.31377400	-0.07081500
C	-2.12026400	0.58492500	-1.13695700
C	-3.43952100	0.86713000	-1.51006900

C	-4.50972400	0.26740400	-0.85155800
C	-4.24308900	-0.60672200	0.22180000
C	-2.93765500	-0.87807700	0.60858000
C	-1.07395100	1.17408800	-1.89843700
N	-0.21036300	1.64344700	-2.49936100
C	-3.68863200	1.77916800	-2.58427400
N	-3.87960400	2.52020900	-3.44039000
C	-5.85188700	0.55132700	-1.23619600
N	-6.93463200	0.78140700	-1.54524200
C	-5.33534900	-1.18812000	0.93820800
N	-6.21539200	-1.65462900	1.50992500
C	-2.74913900	-1.63478400	1.80806600
N	-2.62707900	-2.19099300	2.80640800
C	0.46529400	0.55389000	0.35747800
C	1.82253900	0.31374400	-0.07072900
C	2.12042700	-0.58426300	-1.13727300
C	3.43968900	-0.86612700	-1.51064400
C	4.50984900	-0.26679500	-0.85164900
C	4.24304100	0.60652100	0.22231500
C	2.93757900	0.87771500	0.60915100
C	1.07415100	-1.17319500	-1.89908100
N	0.21074000	-1.64310400	-2.49983300
C	3.68895300	-1.77727200	-2.58554900
N	3.88006400	-2.51753600	-3.44230400
C	5.85203100	-0.55043900	-1.23636200
N	6.93479600	-0.78037000	-1.54545900
C	5.33528300	1.18728900	0.93934700
N	6.21524700	1.65320600	1.51166600
C	2.74888400	1.63357800	1.80911100
N	2.62682100	2.18910800	2.80783000
C	0.03175900	1.83907200	0.84454800
C	-0.88009100	1.88108300	1.92915300
C	-1.20786500	3.05615000	2.54550500
C	-0.65452900	4.25909700	2.08085300
C	0.19270300	4.27069700	0.99911700
C	0.52833600	3.08282600	0.35265000
O	1.33051100	3.18625700	-0.71080300
H	0.60111100	5.19234200	0.60757400
H	-0.90892200	5.19139800	2.56894400
H	-1.87494500	3.05699500	3.39688900
H	-1.25986300	0.94583000	2.32184000
O	-1.33009000	-3.18647600	-0.71196400
H	-0.60136100	-5.19264500	0.60623000
H	0.90816900	-5.19217000	2.56807800

H	1.87425400	-3.05804100	3.39652200
H	1.25947200	-0.94661000	2.32186800
H	-1.10313600	-2.53400600	-1.39842200
H	1.10320200	2.53433200	-1.39760300

TD-LC-DFTB2, not converged:

TPE (CN)₅CF₃ in S₀

ω B97xD, E = -2599.20297 a.u.:

C	-0.68740200	2.30140300	1.42045200
C	0.16474100	1.93193600	0.37859300
C	0.67651300	2.95480600	-0.43929700
C	0.28357500	4.26998600	-0.23000700
C	-0.59446100	4.60279500	0.78692400
C	-1.07000000	3.61342700	1.62717400
C	0.48154800	0.47284900	0.24305700
C	1.93410000	0.10896700	0.26119500
C	2.55656800	-0.60822300	-0.76784700
C	3.93514700	-0.85385000	-0.74484200
C	4.71821200	-0.39741100	0.31694400
C	4.10594900	0.28327800	1.36958000
C	2.72873300	0.52422000	1.33841000
C	1.82615200	-1.12672100	-1.88164900
N	1.31207200	-1.59430400	-2.79500100
C	4.55320800	-1.57801100	-1.81157000
N	5.05762100	-2.16453400	-2.66000300
C	6.12607000	-0.64029400	0.33612300
N	7.25715500	-0.83681000	0.35562000
C	4.88541800	0.71979000	2.48559800
N	5.51141400	1.06915200	3.38255400
C	2.13282700	1.13591700	2.48698800
N	1.66769600	1.57348900	3.44158700
C	1.70444000	2.72756500	-1.52887900
C	-0.48156200	-0.47285100	0.24300900
C	-1.93411300	-0.10897200	0.26116700
C	-2.55657300	0.60833300	-0.76779900
C	-3.93515300	0.85394700	-0.74478300
C	-4.71823100	0.39736700	0.31693400
C	-4.10597700	-0.28344500	1.36949600
C	-2.72875700	-0.52436300	1.33832000
C	-1.82614700	1.12695400	-1.88153800
N	-1.31205400	1.59463100	-2.79483500
C	-4.55320500	1.57823700	-1.81142900

N	-5.05760700	2.16485900	-2.65980100
C	-6.12609300	0.64022300	0.33611400
N	-7.25718200	0.83671600	0.35561000
C	-4.88546100	-0.72011900	2.48544000
N	-5.51147300	-1.06961000	3.38233500
C	-2.13285900	-1.13621800	2.48681900
N	-1.66771600	-1.57391100	3.44135600
C	-0.16475900	-1.93194900	0.37843300
C	-0.67648100	-2.95474500	-0.43958000
C	-0.28353500	-4.26994100	-0.23040100
C	0.59444700	-4.60284000	0.78654600
C	1.06992200	-3.61355000	1.62692500
C	0.68732400	-2.30151000	1.42030900
C	-1.70437000	-2.72740500	-1.52917700
H	-0.66718300	-5.04503900	-0.87820000
H	0.88491300	-5.63524300	0.92952100
H	1.72239400	-3.85861200	2.45477100
H	1.01656800	-1.54553100	2.11927300
H	0.66726300	5.04514400	-0.87771000
H	-0.88492600	5.63518700	0.92998300
H	-1.72252200	3.85841400	2.45500300
H	-1.01669700	1.54535900	2.11932100
F	1.74311400	3.72976500	-2.40262300
F	2.94646000	2.63075600	-0.99372400
F	1.50058900	1.60493900	-2.22255700
F	-1.74294300	-3.72947700	-2.40307100
F	-2.94642200	-2.63075300	-0.99406700
F	-1.50055500	-1.60466100	-2.22267300

TD-LC-DFTB2, E = -118.05605 a.u.:

C	-0.7245075	2.3138191	1.4352790
C	0.1575075	1.9394365	0.3968056
C	0.6911995	2.9646583	-0.4357048
C	0.2933830	4.2975930	-0.2197910
C	-0.6026484	4.6395455	0.7948858
C	-1.1018560	3.6418153	1.6350650
C	0.4924533	0.4814775	0.2581121
C	1.9503961	0.1220158	0.2701807
C	2.5662668	-0.6314615	-0.7642025
C	3.9549071	-0.9070282	-0.7324831
C	4.7568116	-0.4334839	0.3297442
C	4.1559662	0.3101859	1.3697938
C	2.7680955	0.5830942	1.3366286
C	1.8230835	-1.1378009	-1.8949345

N	1.2871562	-1.5823535	-2.8078161
C	4.5559019	-1.6800538	-1.7935389
N	5.0379301	-2.3037700	-2.6282584
C	6.1716518	-0.7164877	0.3593664
N	7.2960477	-0.9467387	0.3879586
C	4.9560235	0.7868219	2.4728093
N	5.5940511	1.1609666	3.3509782
C	2.1975596	1.2947778	2.4577075
N	1.7709044	1.8296770	3.3803002
C	1.7051837	2.7265200	-1.5388074
C	-0.4924578	-0.4814807	0.2580517
C	-1.9504006	-0.1220226	0.2701306
C	-2.5662553	0.6315548	-0.7641903
C	-3.9548971	0.9071132	-0.7324667
C	-4.7568169	0.4334644	0.3297018
C	-4.1559870	-0.3103051	1.3696900
C	-2.7681163	-0.5832069	1.3365190
C	-1.8230548	1.1380144	-1.8948563
N	-1.2871129	1.5826733	-2.8076788
C	-4.5558776	1.6802375	-1.7934582
N	-5.0378945	2.3040291	-2.6281272
C	-6.1716590	0.7164576	0.3593221
N	-7.2960584	0.9466959	0.3879029
C	-4.9560652	-0.7870487	2.4726445
N	-5.5941136	-1.1612768	3.3507606
C	-2.1975947	-1.2949979	2.4575428
N	-1.7709557	-1.8299773	3.3800896
C	-0.1575176	-1.9394544	0.3966019
C	-0.6912003	-2.9645897	-0.4360217
C	-0.2933828	-4.2975460	-0.2202409
C	0.6026404	-4.6396020	0.7944087
C	1.1018301	-3.6419592	1.6347019
C	0.7244797	-2.3139434	1.4350511
C	-1.7051694	-2.7263444	-1.5391153
H	-0.6993816	-5.0869308	-0.8697313
H	0.8952664	-5.6891587	0.9385409
H	1.7824730	-3.8964761	2.4595117
H	1.0882529	-1.5529626	2.1409990
H	0.6993894	5.0870452	-0.8691960
H	-0.8952679	5.6890893	0.9391306
H	-1.7825103	3.8962467	2.4598908
H	-1.0882959	1.5527648	2.1411396
F	1.7856622	3.7876008	-2.4144969
F	2.9917803	2.5642371	-0.9956785

F	1.4577277	1.5979322	-2.2915386
F	-1.7856313	-3.7873400	-2.4149095
F	-2.9917747	-2.5641190	-0.9959908
F	-1.4577061	-1.5976826	-2.2917332

TPE(CN)₅CF₃ in S₁

ω B97xD, E = -2599.08416 a.u.:

C	-0.91318900	2.07033600	1.55940100
C	0.05966400	1.89641500	0.54697100
C	0.57567600	3.06845600	-0.06752700
C	0.12238100	4.30806700	0.34318700
C	-0.82422600	4.44118900	1.35286900
C	-1.33819900	3.31362600	1.96869700
C	0.48323400	0.53578500	0.24515500
C	1.88841500	0.24892500	0.08791500
C	2.38531400	-0.67266800	-0.87778300
C	3.72295100	-1.06670200	-0.88534400
C	4.63018000	-0.54578000	0.04244900
C	4.17245700	0.39107600	0.98397800
C	2.83673000	0.77823700	1.00897400
C	1.56383800	-1.12482600	-1.94982000
N	0.96228100	-1.49091900	-2.85852400
C	4.18048100	-2.01325700	-1.85590800
N	4.54862700	-2.78772400	-2.61949800
C	5.99199500	-0.96166000	0.03986200
N	7.08997700	-1.30204100	0.04317900
C	5.08584700	0.91968100	1.94871500
N	5.82164700	1.34065400	2.72351500
C	2.42273800	1.61912900	2.08879600
N	2.10638100	2.25882200	2.99007700
C	1.63194600	3.10645800	-1.16668800
C	-0.48318700	-0.53584900	0.24509900
C	-1.88835900	-0.24903100	0.08808200
C	-2.38532000	0.67294800	-0.87728000
C	-3.72291900	1.06710200	-0.88455100
C	-4.63010200	0.54594100	0.04314200
C	-4.17236700	-0.39136200	0.98425400
C	-2.83668100	-0.77865700	1.00900200
C	-1.56396600	1.12526800	-1.94933400
N	-0.96252600	1.49151100	-2.85805700
C	-4.18045400	2.01404600	-1.85473900
N	-4.54859600	2.78883600	-2.61800300
C	-5.99186700	0.96196300	0.04086500

N	-7.08981400	1.30246100	0.04443000
C	-5.08573400	-0.92023400	1.94886700
N	-5.82151100	-1.34143100	2.72356700
C	-2.42275300	-1.62002300	2.08848000
N	-2.10663800	-2.26012300	2.98955800
C	-0.05953600	-1.89659300	0.54645200
C	-0.57563100	-3.06838300	-0.06836400
C	-0.12258100	-4.30817900	0.34214100
C	0.82389200	-4.44164200	1.35186400
C	1.33795200	-3.31427100	1.96801600
C	0.91314300	-2.07083800	1.55898000
C	-1.63186400	-3.10613500	-1.16756500
H	-0.50336300	-5.19658400	-0.14169700
H	1.15155600	-5.42926200	1.64896800
H	2.05869600	-3.40210400	2.76996500
H	1.27854600	-1.19663800	2.07793900
H	0.50305500	5.19663800	-0.14041900
H	-1.15206700	5.42870200	1.65013200
H	-2.05907600	3.40116300	2.77056000
H	-1.27862100	1.19597200	2.07805800
F	1.44604100	4.15740200	-1.96587500
F	2.86037900	3.24293000	-0.62320500
F	1.66535600	2.02658700	-1.94287300
F	-1.44581700	-4.15688100	-1.96699100
F	-2.86025800	-3.24278700	-0.62409800
F	-1.66535700	-2.02609100	-1.94352200

TD-LC-DFTB2, E = -117.95692 a.u.:

C	-0.8826623	2.1272630	1.5740340
C	0.0922707	1.9131109	0.5559518
C	0.6102453	3.0658118	-0.1283877
C	0.1065266	4.3325184	0.2021944
C	-0.8691415	4.5089970	1.1932137
C	-1.3521663	3.3960429	1.8921375
C	0.4958664	0.5221320	0.2699709
C	1.9172816	0.2006814	0.1071781
C	2.3944328	-0.7275254	-0.8842881
C	3.7467395	-1.1229485	-0.9170349
C	4.6787072	-0.6054174	0.0205321
C	4.2300842	0.3317943	0.9944875
C	2.8802925	0.7279325	1.0360657
C	1.5409232	-1.1916267	-1.9489151
N	0.9130105	-1.5646151	-2.8368478
C	4.1888603	-2.0654346	-1.9174633

N	4.5400785	-2.8300218	-2.6990249
C	6.0540318	-1.0229456	-0.0094997
N	7.1523787	-1.3645890	-0.0275325
C	5.1603137	0.8549516	1.9654917
N	5.9043242	1.2622679	2.7400518
C	2.4684844	1.5916674	2.1178439
N	2.1727378	2.2501833	3.0129615
C	1.6853598	3.0426774	-1.2064801
C	-0.4959187	-0.5221197	0.2699203
C	-1.9173040	-0.2006780	0.1071215
C	-2.3944276	0.7276384	-0.8842540
C	-3.7467393	1.1230745	-0.9169844
C	-4.6787242	0.6054279	0.0205360
C	-4.2300902	-0.3318866	0.9943938
C	-2.8803240	-0.7280104	1.0359343
C	-1.5408947	1.1918462	-1.9488177
N	-0.9129325	1.5649194	-2.8367066
C	-4.1888253	2.0656583	-1.9173373
N	-4.5400498	2.8303407	-2.6988546
C	-6.0540644	1.0229941	-0.0095210
N	-7.1524236	1.3646050	-0.0275082
C	-5.1603714	-0.8551126	1.9652996
N	-5.9043410	-1.2625376	2.7398187
C	-2.4685392	-1.5918602	2.1176284
N	-2.1727491	-2.2504380	3.0126307
C	-0.0923212	-1.9131573	0.5557241
C	-0.6102238	-3.0658580	-0.1286900
C	-0.1065409	-4.3325567	0.2017384
C	0.8691172	-4.5091488	1.1927675
C	1.3521266	-3.3962661	1.8918054
C	0.8826439	-2.1274804	1.5738259
C	-1.6853358	-3.0425378	-1.2067916
H	-0.4824843	-5.2134503	-0.3388583
H	1.2370395	-5.5178528	1.4257916
H	2.0904818	-3.5217095	2.6959691
H	1.2295592	-1.2734866	2.1736336
H	0.4825299	5.2135374	-0.3383325
H	-1.2370877	5.5177574	1.4263168
H	-2.0905036	3.5214442	2.6962739
H	-1.2295518	1.2733333	2.1736989
F	1.5796703	4.1281930	-2.0520722
F	2.9567984	3.1104918	-0.6265909
F	1.6773773	1.9143252	-1.9967557
F	-1.5796446	-4.1279206	-2.0525061

F	-2.9567720	-3.1103983	-0.6269529
F	-1.6773241	-1.9140713	-1.9969551

TPE (OH) (CHO) in S_0

ω B97xD, E = -1379.89665 a.u.:

C	-1.75646600	2.32941000	-0.79743200
C	-1.31519100	1.49011900	0.23198200
C	-2.05369200	1.42604600	1.41232000
C	-3.19773400	2.18390100	1.59069300
C	-3.61725500	3.02440800	0.56713800
C	-2.90682000	3.09432000	-0.61665400
C	-0.06449500	0.69461600	0.09719600
C	1.21579100	1.45330800	0.18453300
C	2.21040800	1.38719300	-0.80345000
C	3.45057700	1.98415300	-0.59105800
C	3.69740900	2.70742900	0.56216800
C	2.69739400	2.82442900	1.51505400
C	1.47460800	2.19923100	1.32761400
C	1.99759300	0.77762500	-2.12879200
C	-0.09290000	-0.64125800	-0.00544800
C	-1.38302300	-1.34409800	-0.25699600
C	-1.96228700	-1.20509200	-1.51345900
C	-3.12953500	-1.87777400	-1.84447600
C	-3.74288600	-2.71455900	-0.92484300
C	-3.18335200	-2.85621700	0.33145300
C	-2.01664900	-2.17534200	0.67978300
C	1.13988600	-1.47935600	-0.05632900
C	1.40996200	-2.22554600	-1.20444400
C	2.60514700	-2.90416300	-1.36355300
C	3.55516000	-2.85250300	-0.35079000
C	3.29111700	-2.16040700	0.81603400
C	2.08241500	-1.49015800	0.98240300
O	1.88422100	-0.85209500	2.15439700
O	-1.13177400	2.43315200	-1.98672300
C	-1.57795200	-2.31362500	2.07585000
O	0.93794700	0.72541400	-2.71416900
O	-0.70347500	-1.68785300	2.63075100
H	4.00440700	-2.13562800	1.62969600
H	4.50023500	-3.36974900	-0.46359500
H	2.79698700	-3.45996600	-2.27227900
H	0.67656300	-2.23451500	-2.00197200
H	-3.22922600	3.73364000	-1.42854500
H	-4.51024100	3.62553300	0.68859800

H	-3.75300800	2.12229800	2.51766800
H	-1.70732600	0.76483200	2.19849800
H	-0.42519700	1.77233100	-2.10407600
H	0.93124200	-0.81720100	2.32938900
H	0.71157400	2.26531400	2.09305000
H	2.87623100	3.38676200	2.42301100
H	4.65955800	3.17880800	0.71529100
H	4.21757800	1.89780500	-1.35286200
H	-1.48489800	-0.55751800	-2.23877300
H	-3.56064900	-1.74453900	-2.82903400
H	-4.65217300	-3.24213000	-1.18199900
H	-3.66190300	-3.49212900	1.06856900
H	2.90951500	0.39608000	-2.62125500
H	-2.15801000	-3.05551100	2.65759500

TD-LC-DFTB2, E = -82.68588 a.u.:

C	0.8202325	-2.5688433	-0.8600154
C	0.0998404	-1.8840249	0.1554359
C	-0.1151174	-2.5478566	1.3836059
C	0.3952957	-3.8342793	1.6201014
C	1.1368832	-4.4836193	0.6175136
C	1.3447938	-3.8558072	-0.6184419
C	-0.4017468	-0.4585184	-0.0190250
C	-1.9054802	-0.2686143	-0.0230159
C	-2.6532438	0.0098067	-1.2036582
C	-4.0554767	0.1959453	-1.1018010
C	-4.7171979	0.1059044	0.1274790
C	-3.9779917	-0.1778015	1.2886977
C	-2.5915828	-0.3624425	1.2093052
C	-2.0439764	0.1224627	-2.5573274
C	0.4441657	0.6105982	-0.0260451
C	1.9493488	0.4377774	-0.0241378
C	2.6395976	0.6393605	-1.2413335
C	4.0265351	0.4664750	-1.3327575
C	4.7631364	0.0845277	-0.1983758
C	4.0981945	-0.1123302	1.0166357
C	2.6955670	0.0639608	1.1312612
C	-0.0763912	2.0310320	-0.2000786
C	0.0344846	2.6652343	-1.4571002
C	-0.4903283	3.9490113	-1.6777947
C	-1.1412293	4.6241343	-0.6303882
C	-1.2483285	4.0234774	0.6316755
C	-0.7107908	2.7387437	0.8557202
O	-0.8272798	2.2101597	2.1017268

O	1.0314104	-2.0168897	-2.0834213
C	2.0883258	-0.1488659	2.4742676
O	-0.8656896	-0.0679971	-2.8257138
O	0.9327870	0.1103591	2.7813039
H	-1.7434599	4.5431541	1.4524175
H	-1.5592558	5.6188171	-0.7974266
H	-0.3975737	4.4137053	-2.6604027
H	0.5314154	2.1368733	-2.2767058
H	1.9080354	-4.3565667	-1.4064437
H	1.5456964	-5.4797351	0.7982366
H	0.2216814	-4.3209633	2.5808280
H	-0.6791939	-2.0375358	2.1706757
H	0.4812947	-1.2061311	-2.2143328
H	-0.3000584	1.3786231	2.1977023
H	-2.0237036	-0.5807610	2.1182815
H	-4.4814206	-0.2507677	2.2545280
H	-5.7967487	0.2549051	0.1824179
H	-4.6238904	0.4143773	-2.0099108
H	2.0715927	0.9311963	-2.1300859
H	4.5321189	0.6235851	-2.2873480
H	5.8431463	-0.0571661	-0.2629115
H	4.6654829	-0.4049057	1.9043734
H	-2.7465136	0.4040157	-3.3812721
H	2.7723702	-0.5700302	3.2528159

TPE(OH)(CHO) in S_1

$\omega B97xD$, $E = -1379.78520$ a.u.:

C	1.73811700	2.37041600	0.70288300
C	1.32125600	1.47502200	-0.30017900
C	2.11942600	1.29487500	-1.43329100
C	3.26922800	2.03350000	-1.61982000
C	3.65189400	2.95069300	-0.64238400
C	2.90596700	3.11109100	0.50702300
C	0.05626800	0.74983400	-0.13971100
C	-1.16960200	1.52275800	-0.08043400
C	-2.16341500	1.25319300	0.91069600
C	-3.45386500	1.79373700	0.72592200
C	-3.70498000	2.66771800	-0.30072400
C	-2.67824800	3.05164500	-1.18532000
C	-1.42978600	2.48510100	-1.06520000
C	-1.77665600	0.61619600	2.12369800
C	0.06491000	-0.64217800	0.00031900
C	1.33503900	-1.34267100	0.29359000

C	1.99115900	-1.13500200	1.50270300
C	3.15088300	-1.83135900	1.80662900
C	3.67868900	-2.75255400	0.91223000
C	3.04423400	-2.95843700	-0.29844200
C	1.88542600	-2.25441100	-0.62607500
C	-1.14385500	-1.43486600	-0.00669600
C	-1.37393100	-2.36557400	1.02737400
C	-2.58640200	-2.99189700	1.15987600
C	-3.60723300	-2.73313400	0.23371300
C	-3.39503600	-1.89106200	-0.83139200
C	-2.15337900	-1.27473500	-0.99115900
O	-1.93967300	-0.60055900	-2.11704700
O	1.09757900	2.51501400	1.86682400
C	1.38502500	-2.41784900	-1.99864300
O	-0.56844700	0.39405600	2.43303600
O	0.58141300	-1.71176100	-2.56837400
H	-4.15298900	-1.72107600	-1.58403800
H	-4.56885400	-3.21866700	0.34581000
H	-2.76355300	-3.66406800	1.98891700
H	-0.60026600	-2.50428200	1.77087800
H	3.21140800	3.79872900	1.28493900
H	4.55318500	3.53668500	-0.77621900
H	3.86075300	1.90636500	-2.51690900
H	1.79455900	0.58463800	-2.18438100
H	0.45152900	1.78931900	2.03272400
H	-0.98424500	-0.53701400	-2.27273500
H	-0.65047100	2.72643800	-1.77919400
H	-2.87613800	3.77227900	-1.96760900
H	-4.69319200	3.09767500	-0.41129300
H	-4.22879600	1.55773500	1.44684400
H	1.55183400	-0.45008200	2.21577100
H	3.63943200	-1.65880300	2.75757600
H	4.58110500	-3.29829600	1.15571600
H	3.45801600	-3.65759600	-1.01720500
H	-2.56813600	0.32112000	2.82320300
H	1.85106000	-3.25540400	-2.55140400

TD-LC-DFTB2, E = -82.65256 a.u.:

C	0.1999713	-2.8974414	-0.8411264
C	0.1303730	-1.9106287	0.1820560
C	0.5485819	-2.2676736	1.4862712
C	1.0100356	-3.5599178	1.7776333
C	1.0630652	-4.5274202	0.7574128
C	0.6641725	-4.1975954	-0.5438080

C	-0.4286322	-0.5249551	-0.0349599
C	-1.9212452	-0.3970135	-0.1144033
C	-2.5170174	0.1833747	-1.3055960
C	-3.9384556	0.4100900	-1.3126834
C	-4.7233035	0.0189941	-0.2310917
C	-4.1414638	-0.6086037	0.8959430
C	-2.7466857	-0.8084125	0.9432226
C	-1.6664191	0.4377746	-2.4116793
C	0.4247837	0.5900347	0.0080346
C	1.9170583	0.3788633	-0.0909618
C	2.4995555	0.0486387	-1.3347137
C	3.8860750	-0.1125074	-1.4614387
C	4.7235860	0.0589619	-0.3456027
C	4.1623366	0.3817071	0.8956282
C	2.7625180	0.5378043	1.0453269
C	-0.0465771	2.0074724	-0.0312351
C	0.4721522	2.8762578	-1.0298569
C	-0.0236714	4.1728104	-1.1977340
C	-1.0484285	4.6476982	-0.3523705
C	-1.5394860	3.8383263	0.6764879
C	-1.0273951	2.5351003	0.8624058
O	-1.4536746	1.8358392	1.9367543
O	-0.1424856	-2.6217908	-2.1196120
C	2.1961960	0.7985069	2.3947650
O	-0.3957212	0.1187302	-2.3774129
O	1.0080050	0.6787492	2.6661538
H	-2.3098618	4.2065402	1.3544532
H	-1.4475375	5.6540683	-0.4926249
H	0.3701562	4.8082151	-1.9921244
H	1.2368704	2.5005879	-1.7129656
H	0.7061941	-4.9403479	-1.3409312
H	1.4175090	-5.5358904	0.9795440
H	1.3181484	-3.8110294	2.7933372
H	0.4949999	-1.5194432	2.2818938
H	-0.3256051	-1.6502297	-2.2431503
H	-0.8682629	1.0667086	2.1121231
H	-2.2975648	-1.2582625	1.8319119
H	-4.7651731	-0.9258751	1.7321341
H	-5.8019824	0.1874987	-0.2564257
H	-4.3982396	0.8741380	-2.1874675
H	1.8507305	-0.0772645	-2.2047577
H	4.3149406	-0.3702448	-2.4315656
H	5.8034323	-0.0633047	-0.4436306
H	4.8072024	0.5027079	1.7695443

H	-2.0272391	0.8982194	-3.3416573
H	2.9132424	1.0872038	3.2002853

TPE (OH) (COOH) in S_0

$\omega B97xD$, $E = -1530.40940$ a.u.:

C	-1.07399500	2.94261400	-0.59791900
C	-1.02463800	1.85565600	0.28394400
C	-1.97352100	1.76633400	1.30233900
C	-2.94543000	2.73679400	1.46670300
C	-2.97537000	3.81960800	0.59606800
C	-2.05131700	3.92139000	-0.42658600
C	0.03519600	0.81861200	0.16932200
C	1.41729600	1.27335600	0.48902800
C	2.49980000	1.09609200	-0.37837300
C	3.78180000	1.47898100	0.00985800
C	3.99601600	2.05664300	1.24897300
C	2.92328100	2.25970800	2.10302800
C	1.64987300	1.87398100	1.72222900
C	2.29087100	0.61697400	-1.77662100
C	-0.25845500	-0.45901300	-0.11213700
C	-1.63727100	-0.83423700	-0.53338800
C	-2.14464300	-0.33020100	-1.72679100
C	-3.40919200	-0.68277200	-2.16978400
C	-4.18981600	-1.55536600	-1.42771600
C	-3.69124900	-2.08193700	-0.24816200
C	-2.41991000	-1.73056300	0.20070800
C	0.74600900	-1.55817200	-0.14267200
C	0.90403700	-2.29017800	-1.32114700
C	1.89221700	-3.24741800	-1.45454000
C	2.74768300	-3.49156300	-0.38654700
C	2.58094700	-2.81559100	0.80892600
C	1.56679700	-1.87147100	0.95251200
O	1.43533400	-1.28862100	2.16140000
O	-0.22827100	3.10335400	-1.63422400
C	-1.93347800	-2.25185700	1.51382700
O	1.41006700	1.02114600	-2.49496900
O	-1.35925000	-1.58597800	2.33604800
O	-2.19880700	-3.53950200	1.77640200
O	3.18470400	-0.25406500	-2.25531100
H	3.20613700	-3.02578600	1.66713700
H	3.53299500	-4.23251300	-0.47539100
H	2.00962200	-3.78044300	-2.38871800
H	0.26182200	-2.05967300	-2.16294600

H	-2.07149100	4.74908900	-1.12394300
H	-3.72964700	4.58884900	0.71018200
H	-3.67171800	2.65112100	2.26451800
H	-1.93162700	0.91389600	1.97092700
H	0.31226100	2.31539800	-1.82652400
H	0.51236800	-1.02646600	2.29290800
H	0.81461700	2.02424100	2.39490700
H	3.07834700	2.71823800	3.07142200
H	4.99345600	2.36232800	1.53774300
H	4.60975100	1.36607100	-0.68066600
H	-1.53175400	0.34705000	-2.30886100
H	-3.78729800	-0.26873400	-3.09599200
H	-5.18506400	-1.81990800	-1.76100600
H	-4.31791400	-2.73557900	0.34891900
H	-2.54618700	-3.97268000	0.99071100
H	3.66986800	-0.66358000	-1.53059300

TD-LC-DFTB2, E = -90.48081 a.u.:

C	0.4043241	-2.7086847	-1.0518329
C	0.1686365	-1.8820273	0.0784584
C	0.4811243	-2.3871990	1.3597202
C	1.0104359	-3.6776439	1.5250651
C	1.2341218	-4.4876195	0.3977158
C	0.9345805	-4.0059869	-0.8840922
C	-0.4138759	-0.4815696	-0.0463930
C	-1.9221017	-0.3880315	-0.1019822
C	-2.6147390	0.2354222	-1.1796738
C	-4.0249580	0.3439371	-1.1181008
C	-4.7505990	-0.1687541	-0.0354619
C	-4.0668608	-0.8051196	1.0139109
C	-2.6706452	-0.9101943	0.9779596
C	-1.9072255	0.7504645	-2.3997566
C	0.3918567	0.6162763	0.0247563
C	1.8987849	0.4569454	0.0056002
C	2.5314194	0.2614086	-1.2433896
C	3.9238256	0.1393368	-1.3378687
C	4.7154365	0.2164276	-0.1793461
C	4.1003424	0.4064306	1.0639610
C	2.6936382	0.5244580	1.1832575
C	-0.1326391	2.0382231	-0.0530648
C	0.2355988	2.8507967	-1.1495284
C	-0.3041701	4.1353778	-1.3224762
C	-1.2319712	4.6326975	-0.3906525
C	-1.5907594	3.8594851	0.7223827

C	-1.0319527	2.5775799	0.9095233
O	-1.3887452	1.8865934	2.0228522
O	0.1459305	-2.2907991	-2.3164521
C	2.0725223	0.6701478	2.5400624
O	-0.8598983	0.2802360	-2.8365566
O	0.8855821	0.4584480	2.7765219
O	2.8917398	1.0383606	3.5494637
O	-2.4997206	1.7734575	-3.0501947
H	-2.2957989	4.2440123	1.4599250
H	-1.6667341	5.6247821	-0.5275273
H	-0.0126717	4.7364374	-2.1846959
H	0.9301654	2.4594479	-1.8958822
H	1.1098159	-4.6264284	-1.7635024
H	1.6445855	-5.4920996	0.5192330
H	1.2457979	-4.0458586	2.5246736
H	0.3159140	-1.7534146	2.2350082
H	-0.1881348	-1.3555099	-2.3557100
H	-0.7484314	1.1560945	2.2094611
H	-2.1478045	-1.3883591	1.8085094
H	-4.6218269	-1.2116381	1.8612572
H	-5.8375300	-0.0759736	-0.0122724
H	-4.5573691	0.8340440	-1.9414386
H	1.9215074	0.1979938	-2.1466030
H	4.3924768	-0.0166190	-2.3111077
H	5.8006468	0.1229959	-0.2437704
H	4.7210453	0.4565547	1.9680452
H	3.8160790	1.1256807	3.2443704
H	-3.3344099	2.0341670	-2.6181755

TPE (OH) (COOH) in S_1

$\omega B97xD$, $E = -1530.28395$ a.u.:

C	1.26535500	2.87709000	0.49805900
C	1.13162600	1.80199400	-0.40331000
C	2.10028000	1.62288400	-1.39808900
C	3.12537100	2.53001600	-1.56220200
C	3.21240700	3.62487600	-0.70135900
C	2.30304700	3.79327000	0.32234500
C	-0.00102300	0.88723800	-0.24919900
C	-1.31946900	1.44473000	-0.31023900
C	-2.40328900	0.96287800	0.50354400
C	-3.72392600	1.28896200	0.12881400
C	-3.97314100	2.14224500	-0.91312800
C	-2.89963400	2.75292200	-1.60187200

C	-1.60963500	2.42049200	-1.29393400
C	-2.07913500	0.48395800	1.83872300
C	0.24245600	-0.47888700	0.04254000
C	1.55778900	-0.90564200	0.52662700
C	2.15506600	-0.31196900	1.64167600
C	3.39015200	-0.73636000	2.09473200
C	4.06101200	-1.76582200	1.44560700
C	3.48753300	-2.36330600	0.33617500
C	2.24618300	-1.93885600	-0.13326300
C	-0.79541600	-1.46524900	-0.02325300
C	-0.94964700	-2.42524400	1.00555100
C	-2.04840500	-3.23798500	1.05967800
C	-3.04599900	-3.14276400	0.06938400
C	-2.90702900	-2.27623300	-0.98380700
C	-1.75851400	-1.48139100	-1.07663700
O	-1.56563300	-0.81759400	-2.20457200
O	0.47290600	3.04431500	1.56684300
C	1.72896300	-2.47989100	-1.42892900
O	-1.00278100	0.68863500	2.38436500
O	1.25340500	-1.81057900	-2.30823600
O	1.86370100	-3.80612700	-1.60864200
O	-3.02311200	-0.19531200	2.53305800
H	-3.63419000	-2.22516800	-1.78294900
H	-3.92254200	-3.77608600	0.12907300
H	-2.17416000	-3.92498800	1.88597600
H	-0.22031000	-2.43233500	1.80488200
H	2.38445100	4.61639800	1.02030400
H	4.01157600	4.34589500	-0.82458000
H	3.85310700	2.39533700	-2.35171900
H	2.01103000	0.76383500	-2.05395400
H	-0.09171100	2.26421200	1.73795900
H	-0.64655800	-0.51527200	-2.25110200
H	-0.78707500	2.84163900	-1.85989900
H	-3.10187200	3.46901800	-2.38784900
H	-4.99396400	2.39281300	-1.17211600
H	-4.56516300	0.92881500	0.71201300
H	1.61153500	0.45840600	2.17298200
H	3.82981400	-0.26777900	2.96622100
H	5.03215700	-2.09242500	1.79470000
H	4.03994000	-3.12769200	-0.19980900
H	2.14825500	-4.22103700	-0.78874700
H	-3.73008500	-0.46402300	1.94067200

TD-LC-DFTB2, not converged:

TPE (OH) (CONH₂) in S₀

ω B97xD, E = -1490.68571 a.u.:

C	-1.12136000	2.89785800	-0.65919300
C	-1.05349500	1.83929400	0.25575700
C	-1.99835400	1.76231400	1.27786600
C	-2.98562500	2.72169300	1.41699400
C	-3.03498600	3.77796900	0.51520400
C	-2.11537300	3.86470400	-0.51309800
C	0.02317900	0.81680400	0.16195900
C	1.38842000	1.30528300	0.50772200
C	2.49564900	1.17616000	-0.33530800
C	3.74952000	1.61391400	0.08447100
C	3.91265400	2.19570600	1.32931100
C	2.81409500	2.34717100	2.16149400
C	1.56822500	1.91029200	1.74906800
C	2.33840700	0.65499200	-1.72712900
C	-0.25527100	-0.46216600	-0.12374800
C	-1.63584800	-0.85612800	-0.52212400
C	-2.17224300	-0.36530500	-1.70811100
C	-3.44211900	-0.73486400	-2.12141300
C	-4.19571700	-1.61028700	-1.35514600
C	-3.66670100	-2.12111900	-0.18088700
C	-2.39183200	-1.75253700	0.23903800
C	0.75898700	-1.55072000	-0.17792200
C	0.89182700	-2.28321100	-1.35888600
C	1.88113700	-3.23637200	-1.51725200
C	2.76748200	-3.47266000	-0.47200700
C	2.62455700	-2.79826200	0.72708000
C	1.60255700	-1.86509200	0.89878200
O	1.47876700	-1.30265800	2.11592900
O	-0.28430800	3.03890600	-1.70362800
C	-1.85858000	-2.26299800	1.54198000
O	1.43553100	1.02449300	-2.46684400
O	-1.29289900	-1.54295600	2.35323900
N	-2.07100900	-3.57531400	1.78945500
N	3.29813300	-0.20335700	-2.14498100
H	3.27367800	-3.00365500	1.56876800
H	3.55548100	-4.20850900	-0.58002000
H	1.96919300	-3.78139500	-2.44855100
H	0.21880800	-2.06141400	-2.17891200
H	-2.15120600	4.67146900	-1.23405700
H	-3.80119200	4.53830300	0.60888300

H	-3.70998600	2.64663500	2.21776800
H	-1.94273400	0.92556200	1.96544400
H	0.29782900	2.26802200	-1.85960900
H	0.55311900	-1.04300600	2.25464500
H	0.71124200	2.02612700	2.40096500
H	2.92749400	2.80855900	3.13445400
H	4.88912300	2.54482400	1.64052500
H	4.59352900	1.52996000	-0.58944800
H	-1.57972400	0.31762300	-2.30480000
H	-3.84590700	-0.33033500	-3.04111600
H	-5.19511400	-1.88876300	-1.66470200
H	-4.26504800	-2.78238900	0.43502000
H	-1.69271700	-3.96156500	2.63750400
H	3.80157900	-0.73906000	-1.45737700
H	3.14346500	-0.64448600	-3.03631600
H	-2.37267800	-4.19869200	1.06303100

TD-LC-DFTB2, E = -89.33991 a.u.:

C	0.1713438	-2.8962248	-0.8658684
C	0.1549131	-1.9396914	0.1838802
C	0.6655420	-2.3128221	1.4465050
C	1.1736945	-3.6022553	1.6739027
C	1.1752087	-4.5433986	0.6292767
C	0.6793442	-4.1928428	-0.6342844
C	-0.4091212	-0.5407736	-0.0051664
C	-1.9161150	-0.4322732	0.0355800
C	-2.6747862	0.1476433	-1.0196400
C	-4.0807883	0.2323351	-0.8921497
C	-4.7365860	-0.2502500	0.2487003
C	-3.9877605	-0.8280681	1.2868112
C	-2.5939500	-0.9189724	1.1768989
C	-2.0207577	0.6240597	-2.2878803
C	0.4253224	0.5353822	-0.0792800
C	1.9246107	0.3272877	-0.1542929
C	2.4921152	-0.1198098	-1.3679810
C	3.8754149	-0.3135562	-1.4868028
C	4.7164026	-0.0583245	-0.3910452
C	4.1665214	0.3948235	0.8161934
C	2.7728704	0.5944945	0.9543432
C	-0.0536773	1.9657351	-0.2211547
C	0.2996797	2.7034233	-1.3727945
C	-0.1867498	4.0046871	-1.5857154
C	-1.0446279	4.5913519	-0.6388330
C	-1.3835719	3.8926437	0.5291721

C	-0.8742535	2.5967783	0.7561436
O	-1.1912625	1.9822035	1.9240374
O	-0.2784064	-2.6078608	-2.1131979
C	2.1996371	1.0333272	2.2719002
O	-1.1147503	-0.0137234	-2.8401490
O	1.1104789	0.6159154	2.6898675
N	2.9593344	1.9002574	3.0510865
N	-2.5181891	1.7871506	-2.8681946
H	-2.0311742	4.3489994	1.2782887
H	-1.4375278	5.5963401	-0.8054145
H	0.0926391	4.5498884	-2.4883856
H	0.9388827	2.2415182	-2.1281553
H	0.6840140	-4.9159738	-1.4504099
H	1.5669967	-5.5482306	0.8000000
H	1.5642467	-3.8687275	2.6571032
H	0.6696346	-1.5751304	2.2545461
H	-0.5547970	-1.6583473	-2.2227176
H	-0.5757595	1.2290194	2.1082630
H	-2.0186748	-1.3617678	1.9922641
H	-4.4896292	-1.2069910	2.1791106
H	-5.8228824	-0.1788582	0.3251514
H	-4.6676821	0.6670355	-1.7050809
H	1.8405608	-0.3239931	-2.2198797
H	4.2968799	-0.6674769	-2.4294726
H	5.7931584	-0.2152638	-0.4744658
H	4.8240249	0.5782146	1.6699162
H	2.4791825	2.3393991	3.8283034
H	-2.9594644	2.4730061	-2.2663908
H	-1.9305241	2.2018641	-3.5833995
H	3.6570014	2.4859036	2.6085710

TPE (OH) (CONH₂) in S₁

ω B97xD, E = -1490.65276 a.u.:

C	1.33058200	2.82281800	0.52759500
C	1.17403000	1.76614100	-0.39232600
C	2.14603900	1.57337200	-1.38032100
C	3.20085000	2.45122800	-1.51911400
C	3.31393200	3.52789500	-0.63924700
C	2.39936500	3.70753100	0.37834900
C	0.01525300	0.88112300	-0.24834700
C	-1.28183900	1.47644800	-0.33226600
C	-2.39724900	1.03565900	0.45709400
C	-3.69669800	1.40860300	0.06622600

C	-3.89947500	2.27308600	-0.97836900
C	-2.79261800	2.84557800	-1.64603400
C	-1.52082700	2.46837400	-1.31736300
C	-2.12471400	0.52939000	1.80019000
C	0.22823900	-0.48996700	0.06478500
C	1.54063700	-0.93366300	0.53991800
C	2.15210900	-0.35740400	1.65592200
C	3.38932300	-0.79608800	2.09003000
C	4.04511700	-1.82016400	1.41794300
C	3.45683500	-2.39617700	0.30344500
C	2.21531000	-1.95782700	-0.14754100
C	-0.81697900	-1.46325700	-0.00244500
C	-0.96631600	-2.44351900	1.00870900
C	-2.08510800	-3.22872600	1.07932000
C	-3.11314500	-3.07965800	0.12711000
C	-2.97282400	-2.20227300	-0.91885900
C	-1.79918300	-1.44843300	-1.03643300
O	-1.59216600	-0.80129300	-2.17420400
O	0.53075800	2.99894100	1.58969600
C	1.66858900	-2.47694000	-1.44508500
O	-1.04324300	0.73058800	2.37090200
O	1.20593800	-1.75130400	-2.31367700
N	1.76696100	-3.81638000	-1.62392100
N	-3.13345300	-0.13259200	2.45482600
H	-3.71955400	-2.11648500	-1.69716100
H	-4.00995100	-3.68221200	0.20430600
H	-2.19975700	-3.93887500	1.88826100
H	-0.20924400	-2.49205600	1.78084200
H	2.49931300	4.51607800	1.09092300
H	4.13652200	4.22555000	-0.74227100
H	3.93213900	2.30647500	-2.30374000
H	2.03652300	0.72634200	-2.04856900
H	-0.06479900	2.23549900	1.74414500
H	-0.65303600	-0.56527000	-2.24004900
H	-0.67450700	2.86291200	-1.86685900
H	-2.95452700	3.57145100	-2.43284500
H	-4.90588200	2.56492900	-1.25103400
H	-4.54705500	1.07531000	0.64932800
H	1.62040700	0.41341600	2.19903200
H	3.84328100	-0.34083000	2.96141400
H	5.01827500	-2.15810700	1.75112300
H	3.99179900	-3.15848100	-0.25131000
H	1.40375600	-4.20777900	-2.47583200
H	-3.78453500	-0.66570500	1.90302500

H	-2.85394900	-0.55474900	3.32440900
H	1.99451600	-4.42896900	-0.86252000

TD-LC-DFTB2, E = -89.30195 a.u.:

C	0.1214901	-2.9232122	-0.7417911
C	0.1550262	-1.9246646	0.2706220
C	0.7310467	-2.2504807	1.5198736
C	1.2380763	-3.5350740	1.7708235
C	1.1798779	-4.5181982	0.7661229
C	0.6295054	-4.2140762	-0.4866822
C	-0.4445824	-0.5588262	0.0520659
C	-1.9287041	-0.4499926	0.0411646
C	-2.5830584	0.2438042	-1.0714884
C	-4.0019941	0.5165217	-0.9582791
C	-4.7314563	0.0320860	0.1151047
C	-4.1027064	-0.7397804	1.1355593
C	-2.7155493	-0.9654016	1.0872807
C	-1.8185522	0.5136556	-2.2356858
C	0.3959437	0.5653999	-0.0652654
C	1.8802427	0.3565325	-0.2528965
C	2.3822469	-0.1225866	-1.4836702
C	3.7571384	-0.3116308	-1.6780169
C	4.6600664	-0.0214676	-0.6418501
C	4.1777488	0.4562543	0.5845694
C	2.7936489	0.6502166	0.7998865
C	-0.0865218	1.9821516	-0.0637396
C	0.3481377	2.8668549	-1.0860279
C	-0.1649116	4.1649304	-1.1962492
C	-1.1257904	4.6197445	-0.2697540
C	-1.5313945	3.7922752	0.7829625
C	-0.9961758	2.4913763	0.9131406
O	-1.3337142	1.7730845	2.0042248
O	-0.3643574	-2.6510266	-1.9783095
C	2.2848186	1.0780590	2.1460815
O	-0.5643427	0.1454605	-2.3135136
O	1.1803744	0.7079925	2.5709526
N	3.1119891	1.8587326	2.9426380
N	-2.3644166	1.1170284	-3.3759467
H	-2.2492256	4.1469862	1.5229559
H	-1.5407006	5.6251481	-0.3644880
H	0.1670349	4.8157533	-2.0064533
H	1.0622050	2.5076875	-1.8302857
H	0.5907395	-4.9682329	-1.2732553
H	1.5690667	-5.5197630	0.9600249

H	1.6697368	-3.7688172	2.7451106
H	0.7697774	-1.4852017	2.3007185
H	-0.5445975	-1.6786872	-2.0821239
H	-0.7135713	1.0173596	2.1314459
H	-2.2298615	-1.5041118	1.9045087
H	-4.6916699	-1.1288595	1.9663363
H	-5.8027037	0.2339416	0.1792349
H	-4.4921314	1.0935207	-1.7486039
H	1.6807741	-0.3431330	-2.2911112
H	4.1244796	-0.6872299	-2.6347934
H	5.7311529	-0.1729203	-0.7852774
H	4.8817323	0.6629863	1.3948659
H	2.6822065	2.2891024	3.7534923
H	-3.1825645	1.6952804	-3.2059529
H	-1.6843328	1.5661685	-3.9791662
H	3.8494896	2.4063592	2.5165250

TPE (OH)₂(CHO)₂ in S₀

ω B97xD, E = -1756.99796 a.u.:

C	-1.26456100	2.47783800	-1.10696100
C	-1.14071500	1.56920800	-0.03533800
C	-2.18000700	1.52631700	0.91562000
C	-3.28824000	2.35435600	0.79612600
C	-3.36814600	3.25248800	-0.25279000
C	-2.36394000	3.32457800	-1.19968600
C	0.05179500	0.67254900	0.01371000
C	1.38796700	1.36435200	0.05649200
C	2.40064300	1.14012500	-0.88181100
C	3.64384700	1.75726300	-0.77690300
C	3.88778700	2.70187200	0.19961900
C	2.88941900	2.96753100	1.11601800
C	1.68269300	2.27472200	1.08522800
C	2.21908400	0.31856400	-2.10187300
C	-0.05187900	-0.67253300	0.01390800
C	-1.38805900	-1.36431000	0.05694300
C	-2.40042600	-1.14055100	-0.88181800
C	-3.64358000	-1.75796700	-0.77716900
C	-3.88772200	-2.70212400	0.19965400
C	-2.88967500	-2.96723200	1.11662200
C	-1.68311500	-2.27430500	1.08597500
C	1.14067000	-1.56918500	-0.03505700
C	1.26474400	-2.47811200	-1.10640600
C	2.36430600	-3.32467300	-1.19877500

C	3.36841200	-3.25222700	-0.25182400
C	3.28826200	-2.35385900	0.79688100
C	2.17989900	-1.52596500	0.91601700
O	2.18045400	-0.67322900	1.96202400
O	-0.34526300	2.57972600	-2.08863000
C	-0.87256200	-2.44625800	2.30958900
O	1.26808300	0.42642800	-2.83621600
O	-0.20075600	-1.58882800	2.82739000
C	0.87209200	2.44727700	2.30877000
C	-2.21871400	-0.31940400	-2.10211300
O	0.20012900	1.59020900	2.82689300
O	-1.26765300	-0.42765600	-2.83636900
O	0.34547800	-2.58057700	-2.08801200
O	-2.18075800	0.67370700	1.96171300
H	4.05818700	-2.28967600	1.55343900
H	4.22809300	-3.90649200	-0.33162700
H	2.41551400	-4.00764000	-2.03576200
H	-2.41506400	4.00718100	-2.03696200
H	-4.22776100	3.90682600	-0.33276500
H	-4.05826400	2.29054000	1.55261700
H	0.11018500	1.74012400	-2.28608900
H	1.27377500	-0.48156300	2.24254600
H	3.06033800	3.68723900	1.90904600
H	4.84011900	3.21203800	0.25234600
H	4.41053900	1.51778300	-1.50548800
H	-4.41004400	-1.51891900	-1.50612600
H	-4.83996800	-3.21248000	0.25223100
H	-3.06086000	-3.68658000	1.90991300
H	3.04959000	-0.36191900	-2.35784500
H	-0.99429900	-3.42442500	2.81078600
H	0.99394200	3.42576000	2.80936100
H	-3.04901100	0.36118300	-2.35836900
H	-0.11027600	-1.74115700	-2.28588700
H	-1.27412100	0.48194300	2.24240600

TD-LC-DFTB2, E = -102.28456 a.u.:

C	0.6951937	-2.4776962	-1.5529434
C	0.7733583	-1.7173214	-0.3473940
C	1.7828382	-2.0789464	0.5960963
C	2.6781501	-3.1376839	0.3292465
C	2.5624290	-3.8776860	-0.8560682
C	1.5692616	-3.5594971	-1.7935524
C	-0.1982177	-0.5643944	-0.1293663
C	-1.6724778	-0.9437620	-0.1405862

C	-2.6188955	-0.3536177	-1.0257081
C	-3.9756964	-0.7437656	-0.9816651
C	-4.4093564	-1.7494492	-0.1088026
C	-3.4865753	-2.3456625	0.7610002
C	-2.1371069	-1.9337559	0.7729422
C	-2.2371465	0.6436361	-2.0825753
C	0.2276003	0.7231857	0.0734398
C	1.7044646	1.0828251	0.1596388
C	2.6357116	0.7962715	-0.8789007
C	3.9991137	1.1316720	-0.7252555
C	4.4534866	1.7981420	0.4196135
C	3.5441229	2.1018492	1.4415930
C	2.1883509	1.7265562	1.3345646
C	-0.7386292	1.8862466	0.2530759
C	-0.6701838	2.9971920	-0.6409857
C	-1.5338104	4.1044033	-0.4991095
C	-2.5055647	4.1082123	0.5120619
C	-2.6124700	3.0230646	1.3932239
C	-1.7285987	1.9275529	1.2815622
O	-1.8755344	0.9344411	2.1921728
O	-0.2052030	-2.1865852	-2.5250236
C	1.3231081	1.9161367	2.5477318
O	-1.3579132	0.4331563	-2.8974160
O	0.7218366	0.9931684	3.0696657
C	-1.2613116	-2.4801955	1.8629962
C	2.2287278	0.2021694	-2.1967342
O	-0.6449945	-1.7574944	2.6275096
O	1.3245727	0.6596408	-2.8715536
O	0.2109236	3.0315845	-1.6716811
O	1.9406131	-1.4355268	1.7788049
H	-3.3612229	3.0190845	2.1845423
H	-3.1827755	4.9585984	0.6124587
H	-1.4490219	4.9379427	-1.1954753
H	1.4764788	-4.1217244	-2.7219802
H	3.2496423	-4.7033807	-1.0505603
H	3.4441206	-3.3800426	1.0651400
H	-0.5838309	-1.2761090	-2.4479856
H	-1.1003595	0.3290791	2.2399119
H	-3.8172178	-3.1132210	1.4639896
H	-5.4554902	-2.0581914	-0.0995289
H	-4.6871342	-0.2689809	-1.6607357
H	4.6995833	0.8887480	-1.5272448
H	5.5051087	2.0706805	0.5181277
H	3.8903378	2.6023718	2.3484569

H	-2.8447262	1.5796406	-2.1448064
H	1.2921853	2.9339776	3.0093146
H	-1.2369948	-3.5890459	2.0030366
H	2.8385714	-0.6503227	-2.5841006
H	0.5821449	2.1430240	-1.8983945
H	1.1621839	-0.8896774	2.0345709

TPE(OH)₂(CHO)₂ in S₁

ωB97xD, E = -1756.88732 a.u.:

C	-1.22951500	2.43552100	-1.15651400
C	-1.07779800	1.59340800	-0.01926600
C	-2.12052100	1.57602500	0.94366900
C	-3.24011600	2.37263900	0.78966200
C	-3.33769200	3.21432900	-0.31010400
C	-2.34925600	3.25718700	-1.27192800
C	0.10401100	0.72375200	0.04193300
C	1.41486100	1.36328200	-0.02284200
C	2.43607400	0.99820100	-0.95859000
C	3.73220100	1.52565400	-0.82020900
C	4.02515000	2.50032700	0.09661800
C	3.01305500	2.93505200	0.96178400
C	1.76071800	2.34997000	0.94612900
C	2.14557900	0.30270600	-2.17272000
C	-0.05925100	-0.67419400	0.03829400
C	-1.40275100	-1.31384200	0.10105900
C	-2.47167900	-1.04123200	-0.76454100
C	-3.73318300	-1.58918500	-0.55800900
C	-3.95470700	-2.51758400	0.44023500
C	-2.90556000	-2.83900700	1.27848100
C	-1.66941500	-2.21106200	1.15810600
C	1.08751400	-1.55051000	-0.03429500
C	1.14323500	-2.54457400	-1.06667200
C	2.23424100	-3.38014400	-1.17298000
C	3.31339500	-3.23489200	-0.30367900
C	3.32426700	-2.27254600	0.68050800
C	2.21832200	-1.44538100	0.84352900
O	2.24441300	-0.62065000	1.88027800
O	-0.37478900	2.43786800	-2.17810300
C	-0.81582900	-2.39205200	2.35170300
O	0.99596100	0.15504200	-2.62696400
O	-0.05771700	-1.57666500	2.81624200
C	1.04895500	2.54065200	2.20769700
C	-2.34851100	-0.31505500	-2.05528200

O	0.32440200	1.72208100	2.74700400
O	-1.51230200	-0.58154800	-2.87845700
O	0.17421500	-2.67338600	-1.97811800
O	-2.06165100	0.79340100	2.03534400
H	4.14781000	-2.16802900	1.37250000
H	4.16747500	-3.89246500	-0.41159700
H	2.25258700	-4.10135600	-1.97796700
H	-2.43336400	3.88300300	-2.14967300
H	-4.20954400	3.84884800	-0.41575000
H	-4.00072300	2.34782600	1.55746600
H	0.11219400	1.58271100	-2.28349100
H	1.35300400	-0.32948500	2.13175600
H	3.23609600	3.67802600	1.71923100
H	5.01628800	2.92959200	0.15430200
H	4.49233000	1.19382000	-1.51963600
H	-4.53630000	-1.31787000	-1.23461400
H	-4.92650400	-2.97553200	0.56631000
H	-3.05752500	-3.54390900	2.08842500
H	3.00747700	-0.06877700	-2.74628400
H	-0.99286800	-3.34099400	2.89207700
H	1.29354600	3.47405400	2.74359700
H	-3.13658900	0.42872400	-2.26966900
H	-0.21954700	-1.81835200	-2.24814100
H	-1.14085000	0.73634100	2.34271000

TD-LC-DFTB2, E = -102.25142 a.u.:

C	0.6780199	-2.6413252	-1.1582542
C	0.7717967	-1.6854433	-0.0828325
C	1.7705905	-1.9435140	0.9206156
C	2.6197220	-3.0676365	0.8327359
C	2.4807230	-3.9809626	-0.2200778
C	1.5055988	-3.7785026	-1.2096002
C	-0.1759928	-0.5312041	-0.0217298
C	-1.6310541	-0.8963044	-0.2618119
C	-2.4554675	-0.3308169	-1.2853384
C	-3.7395104	-0.8728182	-1.5221385
C	-4.2408721	-1.9438260	-0.7737397
C	-3.4572239	-2.4816736	0.2540342
C	-2.1713691	-1.9662997	0.5237171
C	-2.0991012	0.8419223	-2.1694963
C	0.2534109	0.7984139	0.2564062
C	1.7171183	1.1331738	0.1053184
C	2.3773466	0.8907439	-1.1756569
C	3.7923771	1.1704752	-1.2673113

C	4.4908008	1.7236382	-0.2032102
C	3.8318123	2.0163288	1.0157407
C	2.4557873	1.7044275	1.1745321
C	-0.6949800	1.9153649	0.4795787
C	-0.5331270	3.1747013	-0.2116103
C	-1.4980698	4.1968723	-0.1015154
C	-2.6324619	4.0153771	0.7017357
C	-2.8011844	2.8297141	1.4319328
C	-1.8396633	1.8034212	1.3499497
O	-2.0205170	0.7435765	2.1564727
O	-0.1857553	-2.4543435	-2.1770868
C	1.8202763	1.9121622	2.5033919
O	-2.5396406	0.9508856	-3.2990677
O	0.8242440	1.3001121	2.8712627
C	-1.4635668	-2.4961766	1.7312565
C	1.6362646	0.4449145	-2.3117509
O	-0.8075929	-1.7905114	2.4833835
O	0.3615073	0.2373475	-2.2873513
O	0.5035935	3.4136413	-1.0340424
O	1.8933161	-1.1878947	2.0231427
H	-3.6580532	2.6983238	2.0914555
H	-3.3793519	4.8080244	0.7735306
H	-1.3527681	5.1198233	-0.6612805
H	1.4014979	-4.4742848	-2.0412848
H	3.1334097	-4.8545450	-0.2714268
H	3.3607990	-3.2273199	1.6149980
H	-0.4416841	-1.5000184	-2.2425712
H	-1.2541702	0.1225226	2.1893012
H	-3.8444856	-3.2966896	0.8696004
H	-5.2317773	-2.3493686	-0.9827364
H	-4.3443673	-0.4377212	-2.3207634
H	4.3060188	0.9554389	-2.2064267
H	5.5562644	1.9383413	-0.3022565
H	4.3869093	2.4442436	1.8514666
H	-1.5094701	1.6763978	-1.7132583
H	2.2974262	2.6447027	3.1957615
H	-1.6082087	-3.5754931	1.9763598
H	2.1578362	0.2581292	-3.2664903
H	1.1340710	2.6540421	-1.0673850
H	1.2087082	-0.4819921	2.1021768

TPE (OH)₂(COOH)₂ in S₀

ωB97xD, E = -2058.02930 a.u.:

C	1.69670700	2.15059700	1.17624700
C	1.41851400	1.28217100	0.11221900
C	2.43479300	1.10713600	-0.83347700
C	3.63987500	1.79099000	-0.74064800
C	3.85776700	2.66290300	0.30628000
C	2.88688700	2.84832800	1.27390100
C	0.07648200	0.63115500	0.05258400
C	-1.07103900	1.60481300	0.01250900
C	-2.15557200	1.62243300	0.89806200
C	-3.17385800	2.56157700	0.75159700
C	-3.11944200	3.53467500	-0.22419900
C	-2.04636800	3.54795700	-1.09564600
C	-1.05106900	2.58639800	-0.98956000
C	-2.36266300	0.68562800	2.05996700
C	-0.08788300	-0.70370700	0.00051600
C	1.07474600	-1.66137400	-0.03160600
C	2.08861700	-1.72436200	0.93320000
C	3.12910400	-2.64089600	0.81070600
C	3.15446300	-3.55551100	-0.22322300
C	2.15306300	-3.51965600	-1.17585100
C	1.14882800	-2.56653000	-1.10009200
C	-1.43552800	-1.34121300	-0.05581800
C	-1.75998400	-2.28697500	0.92794200
C	-2.99167200	-2.90301700	0.99077400
C	-3.95646300	-2.56577100	0.05546400
C	-3.68281300	-1.64499800	-0.93009600
C	-2.43194900	-1.03812800	-1.00443900
O	-2.28234100	-0.14333300	-1.99823300
O	0.73823700	2.27052200	2.14294800
C	0.21688600	-2.51549500	-2.27764800
O	-3.44009600	0.22304900	2.31246400
O	-0.37818700	-3.46467000	-2.69570700
O	0.14990500	-1.32385500	-2.89736000
O	-1.31890800	0.45016500	2.85215400
O	2.23340700	0.23759500	-1.86093400
O	-0.80750000	-2.55000300	1.88184900
C	2.16287800	-0.87019700	2.16820400
C	-0.05239500	2.54802900	-2.10429800
O	3.17996800	-0.32901300	2.51115000
O	1.06484900	-0.78495700	2.91361200
O	0.05786600	1.62591600	-2.86292400
O	0.68431900	3.65834100	-2.28118500
H	-4.41627800	-1.38038600	-1.67865600
H	-4.93160000	-3.03309600	0.10101700

H	-3.20725600	-3.61447300	1.77926800
H	3.06616700	3.50214500	2.11899000
H	4.80000900	3.18964100	0.38088500
H	4.40660600	1.62778000	-1.48870000
H	1.11851500	2.67105300	2.92787400
H	-1.36660900	-0.06702500	-2.29945900
H	-2.00250800	4.28002500	-1.89380300
H	-3.91115800	4.26649900	-0.31536500
H	-4.01119400	2.51329000	1.43520100
H	3.90876500	-2.63384300	1.56126600
H	3.94935300	-4.28705000	-0.28864400
H	2.14600000	-4.21953600	-2.00193300
H	0.78541200	-0.68895800	-2.51800400
H	-0.52774000	0.94525800	2.57795100
H	2.85400900	0.42163700	-2.56917800
H	-1.17673300	-3.13690900	2.54478700
H	0.33531600	-1.32828700	2.55637600
H	0.56330700	4.25240900	-1.53396100

TD-LC-DFTB2, E = -117.88021 a.u.:

C	-0.4400226	-2.7245169	-0.9731333
C	0.0968635	-1.8062211	-0.0336831
C	1.0074330	-2.3329826	0.9214941
C	1.3583408	-3.6985704	0.9334935
C	0.8091903	-4.5740637	-0.0141126
C	-0.0973989	-4.0893758	-0.9697114
C	-0.3389800	-0.3492565	-0.0612863
C	-1.8496856	-0.1632125	-0.0488300
C	-2.5669054	0.5397155	-1.0577210
C	-3.9709606	0.6602808	-0.9584565
C	-4.6800680	0.0716452	0.0966205
C	-3.9831446	-0.6381729	1.0844100
C	-2.5783833	-0.7514372	1.0263104
C	-1.9311815	1.1751852	-2.2762683
C	0.5371955	0.7063968	-0.0389279
C	2.0444614	0.5074801	-0.0386763
C	2.7301068	-0.2176322	-1.0557516
C	4.1291479	-0.3931230	-0.9686175
C	4.8648964	0.1669756	0.0834699
C	4.2007566	0.9099549	1.0694547
C	2.8014414	1.0764403	1.0259769
C	0.0858289	2.1533610	0.0194813
C	0.5934322	3.0754048	-0.9351747
C	0.1999154	4.4228821	-0.9642060

C	-0.7294879	4.8895946	-0.0186770
C	-1.2346701	4.0206181	0.9538768
C	-0.8246238	2.6691960	0.9922869
O	-1.3315201	1.9187508	1.9991401
O	-1.3290828	-2.2706754	-1.9204219
C	2.1625573	1.8629469	2.1513775
O	-2.0506014	2.3602010	-2.5458466
O	2.3928202	3.0454835	2.3470842
O	1.3614972	1.1701716	2.9932225
O	-1.2792404	0.3470834	-3.1182390
O	1.5459351	-1.5165322	1.8772199
O	1.4885757	2.6303278	-1.8849226
C	2.0649500	-0.8084866	-2.2785409
C	-1.8518894	-1.4110415	2.1689827
O	2.1046034	-2.0018084	-2.5486862
O	1.4725176	0.0577292	-3.1224411
O	-1.0215259	-0.8298246	2.8554384
O	-2.1761913	-2.6982526	2.4396934
H	-1.9388542	4.3761218	1.7053743
H	-1.0492957	5.9328788	-0.0399168
H	0.6089763	5.0861273	-1.7274012
H	-0.5278263	-4.7527282	-1.7211512
H	1.0857620	-5.6294045	-0.0085568
H	2.0600219	-4.0592023	1.6871969
H	-1.5306964	-2.9869020	-2.5483061
H	-0.8991242	1.0404834	2.1131528
H	-4.5261903	-1.0847652	1.9206287
H	-5.7648614	0.1713662	0.1545112
H	-4.5099696	1.2188784	-1.7261479
H	4.6411060	-0.9647792	-1.7453503
H	5.9467336	0.0323337	0.1304705
H	4.7675871	1.3596236	1.8871270
H	1.2141915	0.2389869	2.7128477
H	-1.2213487	-0.5751573	-2.7792910
H	2.0979957	-2.0379993	2.4847839
H	1.7246889	3.3697324	-2.4726443
H	1.4589829	0.9808062	-2.7730993
H	-2.8336982	-3.0563577	1.8216491

TPE (OH)₂(COOH)₂ in S₁

ωB97xD, E = -2057.90192 a.u.:

C	1.63401000	2.27250200	1.08644300
C	1.34457500	1.38753000	0.02855800

C	2.35299200	1.21250000	-0.93399200
C	3.54208600	1.92283800	-0.87933500
C	3.76386000	2.81458300	0.15266600
C	2.81402100	2.99362300	1.14138900
C	0.04845400	0.68552800	0.04163900
C	-1.12950400	1.51725100	0.13173800
C	-2.30577600	1.25691200	0.90857300
C	-3.44528700	2.05263700	0.74785100
C	-3.45741800	3.15614200	-0.07127100
C	-2.30960500	3.45337100	-0.81677900
C	-1.19698900	2.64712600	-0.74275600
C	-2.37925700	0.35206100	2.08482100
C	-0.00342600	-0.72624900	-0.01274500
C	1.17905400	-1.61028500	-0.00509500
C	2.26200300	-1.55014300	0.89452200
C	3.35853800	-2.39208100	0.74911200
C	3.38545900	-3.37324500	-0.22440800
C	2.31958600	-3.47506800	-1.10218700
C	1.26192000	-2.58404000	-1.02337100
C	-1.29664600	-1.36587800	-0.10979600
C	-1.64519600	-2.39413700	0.80050900
C	-2.89951400	-2.94267800	0.81975200
C	-3.88936100	-2.48672700	-0.07166300
C	-3.61956800	-1.51108200	-0.98120800
C	-2.32571800	-0.96040000	-1.04812700
O	-2.12317500	-0.12969400	-2.03346700
O	0.71875200	2.36412600	2.09285300
C	0.29719000	-2.61354200	-2.17413900
O	-3.39433900	-0.19103500	2.44746700
O	-0.35154400	-3.57359900	-2.48242100
O	0.26178600	-1.49185900	-2.91071500
O	-1.25789600	0.20955400	2.80543800
O	2.13914200	0.33642200	-1.95182600
O	-0.70281300	-2.72851100	1.72360400
C	2.30877800	-0.68961400	2.11914000
C	-0.27648900	2.71812400	-1.91336200
O	3.29117900	-0.09130600	2.46696800
O	1.21160500	-0.68065800	2.87863100
O	-0.13872000	1.80107800	-2.68707700
O	0.32905400	3.88917100	-2.15623100
H	-4.35426600	-1.16169900	-1.69193000
H	-4.87751700	-2.92395400	-0.02263500
H	-3.15466400	-3.68605300	1.56497100
H	3.00535600	3.65900700	1.97464700

H	4.69602500	3.36254900	0.19637100
H	4.29445000	1.77253200	-1.64501900
H	1.14021300	2.73215600	2.87292600
H	-1.22203400	0.24170600	-2.12625700
H	-2.33709100	4.26107300	-1.54035600
H	-4.34102700	3.77408800	-0.15407400
H	-4.31435700	1.79795200	1.34122500
H	4.17787300	-2.28726500	1.44889700
H	4.22757200	-4.04862500	-0.30040300
H	2.31633400	-4.22313800	-1.88535600
H	0.86210200	-0.81663100	-2.54401600
H	-0.55837500	0.81369100	2.50546600
H	2.80460900	0.46276700	-2.63136600
H	-1.09784500	-3.27992300	2.40260300
H	0.50477300	-1.23593000	2.50866300
H	0.20696900	4.47081400	-1.39903100

TD-LC-DFTB2, E = -117.84566 a.u.:

C	-0.2443570	-2.8002479	-0.7356493
C	0.1272983	-1.8210262	0.2283009
C	1.0203025	-2.2271302	1.2565001
C	1.5131472	-3.5437421	1.3206762
C	1.1308284	-4.4822768	0.3477291
C	0.2506840	-4.1163242	-0.6828093
C	-0.3840556	-0.4214793	0.0655529
C	-1.8227670	-0.1945922	-0.0143294
C	-2.3869819	0.9519549	-0.7549764
C	-3.6857793	1.4275525	-0.4198379
C	-4.4902194	0.7592614	0.4969055
C	-4.0254131	-0.4593405	1.0794084
C	-2.7397084	-0.9405271	0.8375826
C	-1.8589115	1.3647161	-2.0883424
C	0.5425733	0.6767938	-0.0715782
C	2.0249648	0.4662511	-0.1878430
C	2.6402561	-0.3956413	-1.1499054
C	4.0239337	-0.6620987	-1.0709488
C	4.8300124	-0.0466916	-0.1028578
C	4.2525484	0.8699295	0.7905346
C	2.8686586	1.1234986	0.7654617
C	0.0471600	2.0682290	-0.0255966
C	0.5149424	3.0493641	-0.9645058
C	-0.0121328	4.3415214	-0.9899952
C	-1.0165346	4.7207874	-0.0612254
C	-1.4681319	3.8242784	0.9041272

C	-0.9340195	2.5119077	0.9497168
O	-1.2563109	1.7328384	1.9839819
O	-1.0967604	-2.4258469	-1.7416922
C	2.2989556	2.0702037	1.7967623
O	-2.0609990	2.4678256	-2.5942512
O	2.4350911	3.2825908	1.7563560
O	1.6365534	1.4871450	2.8285243
O	-1.1889214	0.4157156	-2.7840908
O	1.3846664	-1.3318094	2.2302109
O	1.4533758	2.6686005	-1.8837065
C	1.9376822	-0.9258428	-2.3774178
C	-2.3035852	-2.1521186	1.6247308
O	1.8547787	-2.1108237	-2.6694348
O	1.4789198	0.0193232	-3.2237047
O	-1.6984341	-2.0968763	2.6839249
O	-2.6940379	-3.3547631	1.1200219
H	-2.2099661	4.1207433	1.6448892
H	-1.4228024	5.7327229	-0.0989520
H	0.3309938	5.0487325	-1.7460894
H	-0.0399150	-4.8345235	-1.4502590
H	1.5190144	-5.5009296	0.3948824
H	2.1869491	-3.8244185	2.1315898
H	-1.1091841	-3.1016777	-2.4420444
H	-0.8811573	0.8290076	1.8799590
H	-4.6809172	-1.0064260	1.7604384
H	-5.4892367	1.1260248	0.7338938
H	-4.0668261	2.3051578	-0.9471727
H	4.4739071	-1.3394850	-1.7995958
H	5.8990717	-0.2587902	-0.0600398
H	4.8769011	1.3793914	1.5274309
H	1.5498816	0.5145673	2.7073360
H	-1.1414375	-0.4372069	-2.2936596
H	1.8946175	-1.7935887	2.9186743
H	1.6476611	3.4063073	-2.4884291
H	1.5188562	0.9224755	-2.8387198
H	-3.1645995	-3.2564918	0.2761367

TPE (OH)₂ (CONH₂)₂ in S₀

ωB97xD, E = -1978.58030 a.u.:

C	2.68263600	-0.95640300	-1.03631900
C	1.91614500	-0.31741500	-0.03846300
C	2.59822200	0.40723100	0.96058900
C	3.98994200	0.46596400	0.95349800

C	4.70959200	-0.20144000	-0.01625200
C	4.06793900	-0.92084900	-1.00904300
C	0.44112300	-0.49878500	-0.05675100
C	0.00911500	-1.94154900	-0.01906600
C	-0.84616600	-2.54504500	-0.94535600
C	-1.18661700	-3.89099300	-0.83952900
C	-0.65629100	-4.67794200	0.16353700
C	0.20186900	-4.10373300	1.08397700
C	0.51272000	-2.75483300	1.00310200
C	-1.32420700	-1.82355300	-2.16187100
C	-0.42918200	0.52791600	-0.04823400
C	-0.00237300	1.97446400	-0.03428300
C	0.85879200	2.58643300	-0.95365600
C	1.15638800	3.94313100	-0.83734500
C	0.58337600	4.73091900	0.13818700
C	-0.26689000	4.14313100	1.05737700
C	-0.53367100	2.78467100	0.98458900
C	-1.90715200	0.31568500	-0.00194600
C	-2.69793100	0.93289400	-0.98438700
C	-4.07645500	0.80868400	-1.02474400
C	-4.70255100	0.00835400	-0.07870200
C	-3.96496800	-0.63094100	0.89275100
C	-2.57529900	-0.46413000	0.96459300
O	-1.99132600	-1.09989300	1.97933800
O	2.12390600	-1.63713700	-2.06213200
C	-1.24401100	2.16598400	2.14629800
O	-0.54481400	-1.26361000	-2.92013400
O	-0.72106400	1.27597700	2.79808800
N	-2.44271300	2.69460100	2.48140500
N	-2.64760900	-1.91290900	-2.41985500
O	2.00605000	1.06078200	1.97360900
O	-2.03374100	1.62505400	-1.95121300
C	1.25187000	-2.13958100	2.15300200
C	1.56856600	1.92975900	-2.11745300
H	-4.43544200	-1.24401500	1.64947300
H	-5.77868800	-0.11249700	-0.10452800
H	-4.64690900	1.30384500	-1.80274000
H	4.61324500	-1.41121600	-1.80352000
H	5.79156100	-0.14654100	-0.01035200
H	4.47697700	1.03730600	1.73199300
H	1.20501500	-1.37926100	-2.25377700
H	-1.07844300	-0.82213400	2.18820000
H	0.61354700	-4.69377800	1.89368900
H	-0.90686200	-5.72874700	0.22762600

H	-1.84336000	-4.32697000	-1.58211200
H	1.85800200	4.36595300	-1.54444600
H	0.81658300	5.78602800	0.20110300
H	-0.68577000	4.72532200	1.86943800
H	-2.95200700	2.25544900	3.22980700
H	-3.28447700	-2.08612700	-1.65877600
H	-2.99559400	-1.37373100	-3.19508000
H	-2.94348500	3.27076000	1.82946600
O	0.68283900	-1.33886000	2.87642400
N	2.50827400	-2.58245100	2.38025600
O	2.74511600	2.16076400	-2.32083000
N	0.81034900	1.18907000	-2.94798600
H	1.08035300	0.81611700	2.14304200
H	-2.65584400	2.07413200	-2.52575300
H	3.04104900	-2.06787300	3.06384100
H	3.02300300	-2.97173000	1.60744700
H	1.28416700	0.66077600	-3.66076500
H	-0.13765000	0.93797200	-2.72380100

TD-LC-DFTB2, E = -115.59276 a.u.:

C	-0.5016202	-3.0775193	-0.7627113
C	0.0505457	-2.1062168	0.1207331
C	0.8847443	-2.5704476	1.1759527
C	1.1140786	-3.9491760	1.3735354
C	0.5203971	-4.8848297	0.5095770
C	-0.2834337	-4.4569280	-0.5561433
C	-0.3359658	-0.6461278	-0.0028841
C	-1.8431084	-0.4125507	0.0204216
C	-2.5512504	0.2709516	-1.0093390
C	-3.9472067	0.4630672	-0.9001445
C	-4.6605420	-0.0308314	0.1987314
C	-3.9751091	-0.7211496	1.2083583
C	-2.5807990	-0.9093666	1.1322950
C	-1.8814478	0.7130194	-2.2792274
C	0.5627003	0.3888853	-0.0111050
C	2.0729185	0.2193465	0.0429977
C	2.8112769	-0.6339881	-0.8281561
C	4.2155393	-0.7208343	-0.6998476
C	4.9114083	0.0410023	0.2459949
C	4.1961093	0.8987855	1.0928619
C	2.7924462	0.9879515	1.0054175
C	0.0985112	1.8362938	-0.0731613
C	0.5517355	2.6429794	-1.1483367
C	0.1348631	3.9792616	-1.3116902

C	-0.7691115	4.5332216	-0.3848275
C	-1.2220894	3.7723102	0.6980519
C	-0.7786351	2.4371353	0.8804141
O	-1.2205505	1.8021208	1.9793602
O	-1.2629815	-2.7152206	-1.8273427
C	2.1002836	1.8749546	2.0175468
O	-1.1368930	-0.0499163	-2.9090239
O	1.4456071	1.4217958	2.9524063
N	2.3418551	3.2544452	1.9066163
N	-2.2024189	1.9668168	-2.7806561
O	1.4312955	-1.6684702	2.0256765
O	1.4020213	2.0896304	-2.0689243
C	-1.8909518	-1.5639008	2.3112449
C	2.2254246	-1.4956390	-1.9302498
H	-1.9058537	4.2031693	1.4288482
H	-1.1082543	5.5632612	-0.5091707
H	0.5033106	4.5637073	-2.1558031
H	-0.7249521	-5.1766868	-1.2445047
H	0.6967621	-5.9511693	0.6640584
H	1.7504684	-4.2745611	2.1976670
H	-1.1851624	-1.7506144	-2.0445154
H	-0.7361417	0.9717985	2.2071888
H	-4.5229403	-1.1073019	2.0704583
H	-5.7393890	0.1166278	0.2655860
H	-4.4789598	0.9850834	-1.6989763
H	4.7649815	-1.3916788	-1.3630494
H	5.9972889	-0.0325528	0.3250582
H	4.7263852	1.4945216	1.8390060
H	1.7028112	3.8451691	2.4283213
H	-2.5242557	2.6840494	-2.1410131
H	-1.6127406	2.3151022	-3.5279971
H	2.5571403	3.6193843	0.9862130
O	-1.2122106	-0.9048765	3.0961463
N	-2.1523504	-2.9197080	2.5256675
O	2.4645082	-2.7044556	-1.9787973
N	1.5489196	-0.8553716	-2.9589125
H	1.9320322	-2.1016621	2.7345495
H	1.6420146	2.7415064	-2.7479045
H	-1.5194432	-3.3881700	3.1655514
H	-2.3957579	-3.4857208	1.7206901
H	0.9918355	-1.4554153	-3.5582819
H	1.1028830	0.0397430	-2.7630721

TPE (OH)₂ (CONH₂)₂ in S₁

$\omega B97xD$, $E = -1978.45330$ a.u.:

C	-2.03199900	-1.97467800	1.01325000
C	-1.55910800	-1.07725600	-0.00189200
C	-2.50921000	-0.62409400	-0.98461100
C	-3.83028100	-1.06779800	-0.93591100
C	-4.21665900	-1.96670100	0.02987800
C	-3.32921900	-2.43363800	0.99873800
C	-0.16822200	-0.67906800	0.03105200
C	0.80179200	-1.76269700	0.08286000
C	1.95231700	-1.82999700	0.91803300
C	2.86991000	-2.87286600	0.77695200
C	2.66808800	-3.89748800	-0.12192900
C	1.53463600	-3.86600900	-0.93753500
C	0.64584800	-2.81740600	-0.85872200
C	2.05940800	-0.98015100	2.11657200
C	0.17511800	0.70303700	0.03759900
C	-0.81975000	1.77623900	0.07865100
C	-1.95120900	1.88642300	0.91839600
C	-2.83858600	2.94959900	0.75809000
C	-2.61963900	3.95408800	-0.16081300
C	-1.51878100	3.86413300	-1.00357000
C	-0.66275300	2.78483500	-0.91155200
C	1.56884500	1.10339300	-0.05253100
C	2.07462200	2.06764500	0.86330200
C	3.40209300	2.44007900	0.88401900
C	4.29691500	1.83479500	0.00132800
C	3.86286900	0.89541500	-0.90288300
C	2.50698800	0.54695500	-0.97216000
O	2.19574900	-0.27299700	-1.96244500
O	-1.25924700	-2.35162300	2.04243100
C	0.22027900	2.52034300	-2.08908700
O	1.07006600	-0.69924100	2.79276300
O	0.08280300	1.50451200	-2.76103800
N	1.09518900	3.48885600	-2.43538200
N	3.30752300	-0.60274200	2.50339900
O	-2.20223300	0.15152800	-2.00563200
O	1.19822800	2.56003800	1.77380200
C	-0.27844200	-2.62255500	-2.01920100
C	-2.30392300	1.01287000	2.09667800
H	4.53558100	0.43932000	-1.61643100
H	5.34313800	2.11451800	0.02603600
H	3.75106900	3.16720700	1.60895600
H	-3.66133800	-3.08095500	1.79814500

H	-5.24450300	-2.30787700	0.05415900
H	-4.51806100	-0.70484600	-1.68659300
H	-0.47072500	-1.78562900	2.14700600
H	1.24432900	-0.43919900	-2.11536500
H	1.39018200	-4.62868200	-1.69387200
H	3.37659500	-4.71156200	-0.19548800
H	3.72152600	-2.91051200	1.44551000
H	-3.70442400	2.97708700	1.40681400
H	-3.31199800	4.78157800	-0.24535900
H	-1.37500900	4.59427900	-1.79174100
H	1.70592300	3.31565000	-3.21590100
H	4.02110800	-0.50181700	1.80097800
H	3.35690500	0.01493900	3.29566500
H	1.33192000	4.21359200	-1.78241900
O	-0.13097400	-1.66768900	-2.77039700
N	-1.20293900	-3.58200400	-2.23893900
O	-3.46639100	0.72329600	2.32336900
N	-1.29532600	0.69069900	2.92812200
H	-1.25623100	0.38006800	-2.13279400
H	1.65392900	3.15164300	2.37535100
H	-1.86407500	-3.43290800	-2.98312200
H	-1.44938500	-4.21369400	-1.49732600
H	-1.49569500	0.01637900	3.64757600
H	-0.32758600	0.80048100	2.66899900

TD-LC-DFTB2, E = -115.55764 a.u.:

C	-0.5431265	-3.0751046	-0.7362176
C	0.0744884	-2.1011244	0.1237685
C	0.9679499	-2.5859680	1.1367471
C	1.1408598	-3.9672665	1.3448295
C	0.4657126	-4.8925055	0.5244624
C	-0.3655327	-4.4586778	-0.5153069
C	-0.3302272	-0.6843675	0.0347297
C	-1.8227095	-0.4229950	0.0377515
C	-2.4599208	0.3578198	-1.0297154
C	-3.8370593	0.7739977	-0.8378693
C	-4.5723486	0.3191777	0.2421051
C	-3.9850079	-0.5453740	1.2102555
C	-2.6056120	-0.8794733	1.1171337
C	-1.7334053	0.5712480	-2.2361046
C	0.5896449	0.3945309	0.0584814
C	2.0897984	0.2474610	-0.0042976
C	2.8183410	-0.6040108	-0.8903123
C	4.2292559	-0.6458017	-0.8216986

C	4.9468253	0.1467872	0.0810794
C	4.2454033	0.9942760	0.9495715
C	2.8394469	1.0475543	0.9196516
C	0.0913239	1.7960867	0.0845116
C	0.5383090	2.6959748	-0.9364532
C	0.0153571	3.9919830	-1.0680963
C	-0.9635797	4.4407294	-0.1542637
C	-1.3865867	3.6167130	0.8884816
C	-0.8649003	2.3035042	1.0355797
O	-1.2403805	1.6393164	2.1242618
O	-1.2587484	-2.6748192	-1.7936007
C	2.1785587	1.9106629	1.9756252
O	-0.5917115	-0.0055900	-2.4111396
O	1.5870873	1.4295804	2.9378133
N	2.3929613	3.2942145	1.8770721
N	-2.2571795	1.3533921	-3.2918104
O	1.5787493	-1.6961482	1.9415186
O	1.4751679	2.2601889	-1.8239782
C	-1.9654255	-1.5995732	2.2707289
C	2.2557347	-1.5116220	-1.9729490
H	-2.1204565	3.9702416	1.6119117
H	-1.3779090	5.4449627	-0.2600875
H	0.3574780	4.6334707	-1.8811839
H	-0.8533455	-5.1750174	-1.1751243
H	0.6086819	-5.9617572	0.6935873
H	1.7963024	-4.3108454	2.1460060
H	-1.1322378	-1.6942744	-1.9658291
H	-0.8609786	0.7277920	2.2601886
H	-4.5714673	-0.8950904	2.0599226
H	-5.6154263	0.6193146	0.3597042
H	-4.2953282	1.4280848	-1.5848287
H	4.7683099	-1.3091466	-1.5009190
H	6.0366357	0.1033045	0.1111826
H	4.7896596	1.6089107	1.6697540
H	1.7820946	3.8692305	2.4475925
H	-2.9120871	2.0743561	-3.0042168
H	-1.5468119	1.7134212	-3.9186477
H	2.5681214	3.6834561	0.9582889
O	-1.0737441	-1.0657527	2.9439645
N	-2.4477860	-2.8611672	2.5962732
O	2.3259358	-2.7371846	-1.8605261
N	1.8553764	-0.9118047	-3.1602044
H	2.0560329	-2.1301616	2.6666425
H	1.6302028	2.9272218	-2.5128675

H	-1.8865799	-3.4195346	3.2285349
H	-2.9504853	-3.3900798	1.8945383
H	1.3410995	-1.5350839	-3.7757786
H	1.3737754	-0.0176032	-3.0627899