

Supplementary Information

The Crucial Role of Non-Conjugated Functional Group on Triplet Manipulation of Heterocycle Aromaticity Hot Exciton Materials

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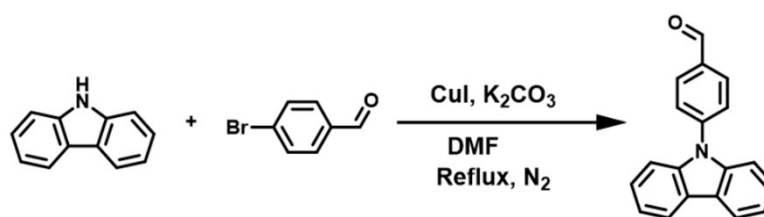
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1. Materials and Methods.

All solvents and reactants required for the experiments and tests were commercially available, with special circumstances mentioned. ^1H NMR and ^{13}C NMR were recorded on a Bruker DRX 600 spectrometer (600 MHz), with tetrahydrofuran- d_8 as deuterated solvent and tetramethylsilane as reference. Mass spectra were analyzed by VJ-ZAB-3F mass spectrometer. Thermogravimetric analysis (TGA) was characterized using a Netzsch TG 209 F3 instrument. Differential scanning calorimetry (DSC) was carried out on a NETZSCH DSC 200 PC apparatus under a nitrogen atmosphere with $10\text{ }^\circ\text{C min}^{-1}$ heating rate. Cyclic voltammetry (CV) adopted CHI600E electrochemical workstation for analysis with calomal, glass carbon and platinum wire electrodes as reference, working and auxiliary electrodes, respectively, standardized for the redox couple ferricinium/ferrocene. HOMO was derived from ionization energy measurements. E_g was acquired from the intersection of absorption-emission spectra. The LUMO levels (eV) of the four compounds were calculated according to HOMO and E_g .

2. Molecular Synthesis.

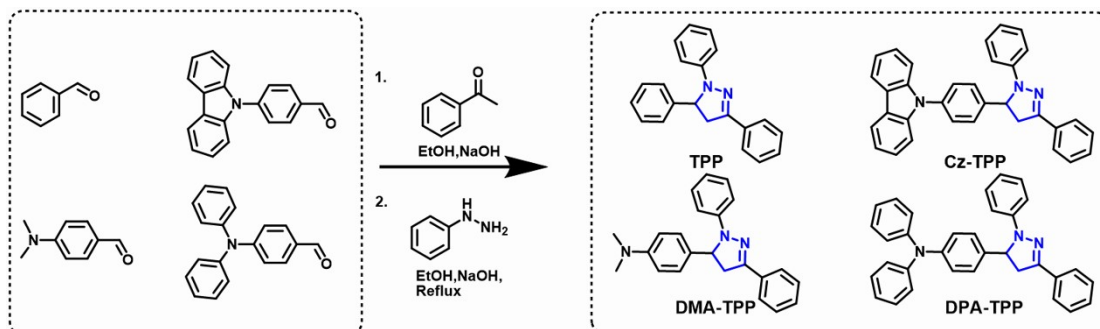
The intermediate and desired compounds were synthesized according to the literature with some minor modifications (**Scheme S1 and S2**).¹



Scheme S1. Molecular synthesis route of 4-(9H-carbazol-9-yl)benzaldehyde.

Synthesis of Intermediate. A mixture of carbazole (2.0 g, 12 mmol), 4-bromobenzaldehyde (2.5 g, 13.5 mmol), potassium carbonate (4.15 g, 30 mmol), and cuprous iodide (0.23 g, 1.2 mmol) was dissolved in *N,N*-dimethylformamide (DMF, 20 mL). The mixed solution was kept stirring under nitrogen atmosphere and then $140\text{ }^\circ\text{C}$ for 20 h. After cooling to room temperature, the inorganic solid was filtered. The filtrate

was poured into ice water for precipitation, and the crude product was obtained after filtration. The crude product was purified by column chromatography (petroleum ether/dichloromethane, v/v = 4:1) to obtain the intermediate 4-(9*H*-carbazol-9-yl)benzaldehyde 2.1 g as white solid (yield 65 %).



Scheme S2. Molecular synthesis route of TPP derivatives.

Synthesis of TPP. Benzaldehyde (2.00 mL, 19.6 mmol) and acetophenone (2.74 mL, 23.5 mmol) were added to 20 mL of anhydrous ethanol, and then the pH was adjusted to 10 by using NaOH. After stirring for 4-8 h at room temperature, the intermediate chalcone derivative was collected via filtration, washing and drying. Under nitrogen atmosphere, phenylhydrazine (1.5 mL, 15.3 mmol) and chalcone derivative (3.8 g, 0.022 mol) were mixed in 20 mL of anhydrous ethanol and refluxed for 12 h. After cooling to room temperature, the solvent was removed under reduced pressure. The obtained solid was further washed in turn with cold ethanol, ice water and dried. The crude product was purified by column chromatography (dichloromethane/petroleum ether, v/v = 1:2) and recrystallization to obtain the product TPP as a white powder (yield 72%). ¹H NMR (600 MHz, C₄D₈O) δ (ppm) = 7.63 (dt, *J* = 8.2, 1.6 Hz, 2H), 7.27–7.14 (m, 7H), 7.10 (ddd, *J* = 6.5, 4.1, 1.7 Hz, 1H), 7.00–6.89 (m, 4H), 6.59–6.52 (m, 1H), 5.24 (dd, *J* = 12.4, 7.0 Hz, 1H), 3.79 (ddd, *J* = 17.1, 12.4, 1.2 Hz, 1H), 3.01 (dd, *J* = 17.1, 7.0 Hz, 1H). ¹³C NMR (101 MHz, C₄D₈O) δ (ppm) = 147.06, 145.46, 143.62, 133.57, 129.28, 128.87, 128.69, 128.65, 127.64, 126.27, 126.05, 119.01, 113.64, 64.73, 43.67. HRMS (MALDI-TOF) calculated for C₂₁H₁₈N₂: 298.147, found: *m/z* 298.113.

Synthesis of Cz-TPP. 4-(9*H*-carbazol-9-yl)benzaldehyde was used as the key reagent instead of benzaldehyde, and the synthesis and post-processing steps were

referred to compound TPP. After recrystallization, the light yellow crystals Cz-TPP were obtained in 67 % yield. ^1H NMR (600 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 8.00 (d, J = 7.8 Hz, 2H), 7.68 (d, J = 7.2 Hz, 2H), 7.54–7.41 (m, 4H), 7.30–7.15 (m, 7H), 7.14–6.97 (m, 6H), 6.65–6.59 (m, 1H), 5.41 (dd, J = 12.6, 6.6 Hz, 1H), 3.88 (dd, J = 17.4, 12.4 Hz, 1H), 3.17 (dd, J = 17.4, 6.6 Hz, 1H). ^{13}C NMR (101 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 147.28, 145.47, 142.91, 141.22, 137.44, 133.51, 129.07, 128.80, 128.75, 127.96, 127.87, 126.15, 126.13, 123.93, 120.44, 120.24, 119.22, 113.62, 110.00, 64.27, 43.70. HRMS (MALDI-TOF) calculated for $\text{C}_{33}\text{H}_{25}\text{N}_3$: 463.205, found: m/z 463.201.

Synthesis of DMA-TPP. 4-dimethylaminobenzaldehyde was used as the key reagent instead of benzaldehyde, and the synthesis and post-processing steps were referred to compound TPP. After recrystallization, the light yellow crystals DMA-TPP were obtained in 65 % yield. ^1H NMR (600 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 7.62 (dd, J = 8.4, 1.2 Hz, 2H), 7.25–7.21 (m, 2H), 7.17–7.13 (m, 1H), 7.03–6.99 (m, 2H), 6.97–6.92 (m, 4H), 6.57–6.51 (m, 3H), 5.12 (dd, J = 12.0, 6.6 Hz, 1H), 3.69 (dd, J = 16.8, 12.0 Hz, 1H), 2.95 (dd, J = 16.8, 6.6 Hz, 1H), 2.77 (s, 6H). ^{13}C NMR (101 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 150.59, 146.90, 145.67, 133.86, 130.94, 128.74, 128.66, 128.45, 126.91, 125.97, 118.75, 113.74, 113.18, 64.54, 43.75, 40.11. HRMS (MALDI-TOF) calculated for $\text{C}_{23}\text{H}_{23}\text{N}_3$: 341.189, found: m/z 341.181.

Synthesis of DPA-TPP. 4-(*N,N*-diphenylamino)benzaldehyde was used as the key reagent instead of benzaldehyde, and the synthesis and post-processing steps were referred to compound TPP. After recrystallization, the light yellow crystals 5DPA-TPP were obtained in 70 % yield. ^1H NMR (600 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 7.64 (d, J = 7.2 Hz, 2H), 7.24 (t, J = 7.2 Hz, 2H), 7.17 (t, J = 7.2 Hz, 1H), 7.09 (dd, J = 13.3, 5.2 Hz, 6H), 7.02–6.95 (m, 4H), 6.94–6.79 (m, 8H), 6.59 (t, J = 6.9 Hz, 1H), 5.24–5.13 (m, 1H), 3.77 (dd, J = 17.1, 12.3 Hz, 1H), 3.03 (dd, J = 17.1, 7.0 Hz, 1H). ^{13}C NMR (101 MHz, $\text{C}_4\text{D}_8\text{O}$) δ (ppm) = 148.29, 147.61, 147.12, 145.64, 137.64, 133.63, 129.56, 128.90, 128.69, 128.64, 127.21, 126.06, 124.69, 124.30, 123.21, 119.02, 113.63, 64.37, 43.71. HRMS (MALDI-TOF) calculated for $\text{C}_{33}\text{H}_{27}\text{N}_3$: 465.220, found: m/z 465.224.

3. Electrochemical and Thermal Properties.

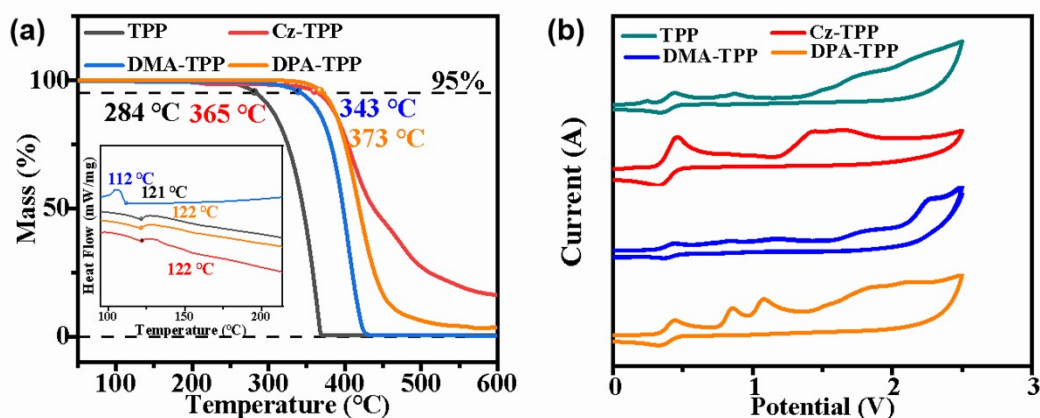


Figure S1. (a) TGA (insert: DSC curves) and CV curves of TPP derivatives.

4. Quantum Chemical Calculation.

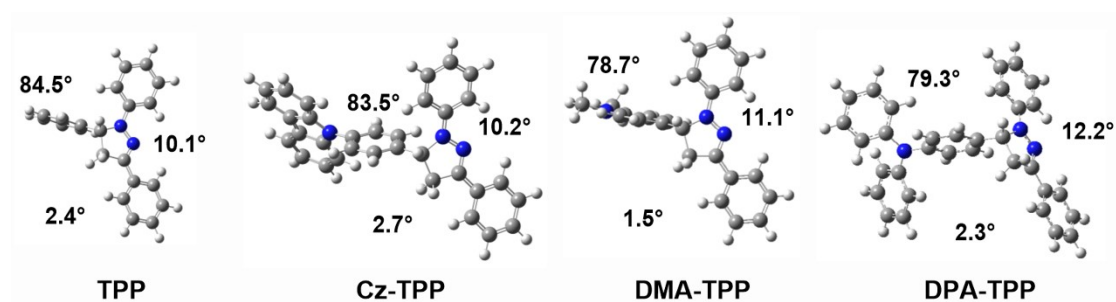


Figure S2. Optimized geometry of TPP, Cz-TPP, DMA-TPP and DPA-TPP species.

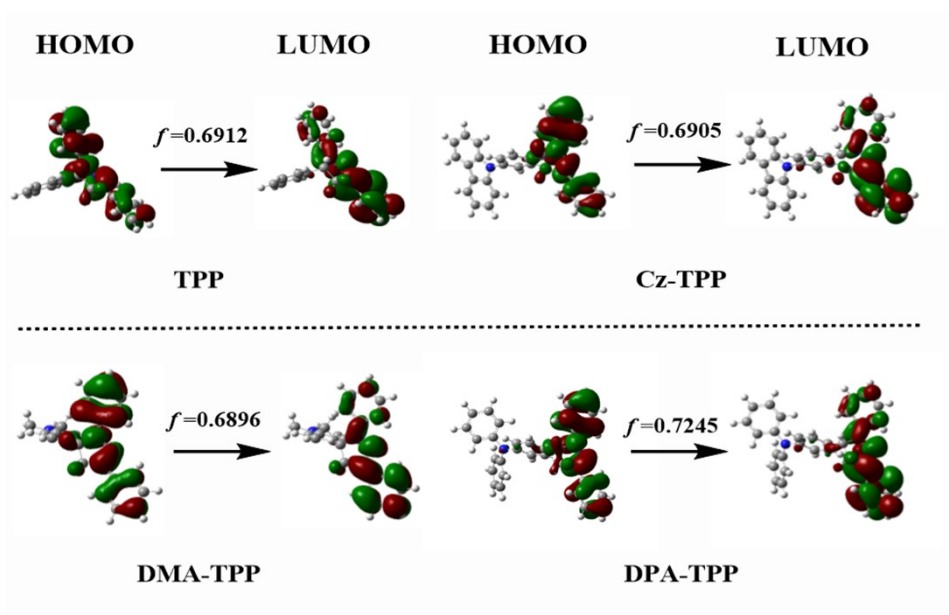


Figure S3. Frontier orbital distribution of TPP, Cz-TPP, DMA-TPP and DPA-TPP species.

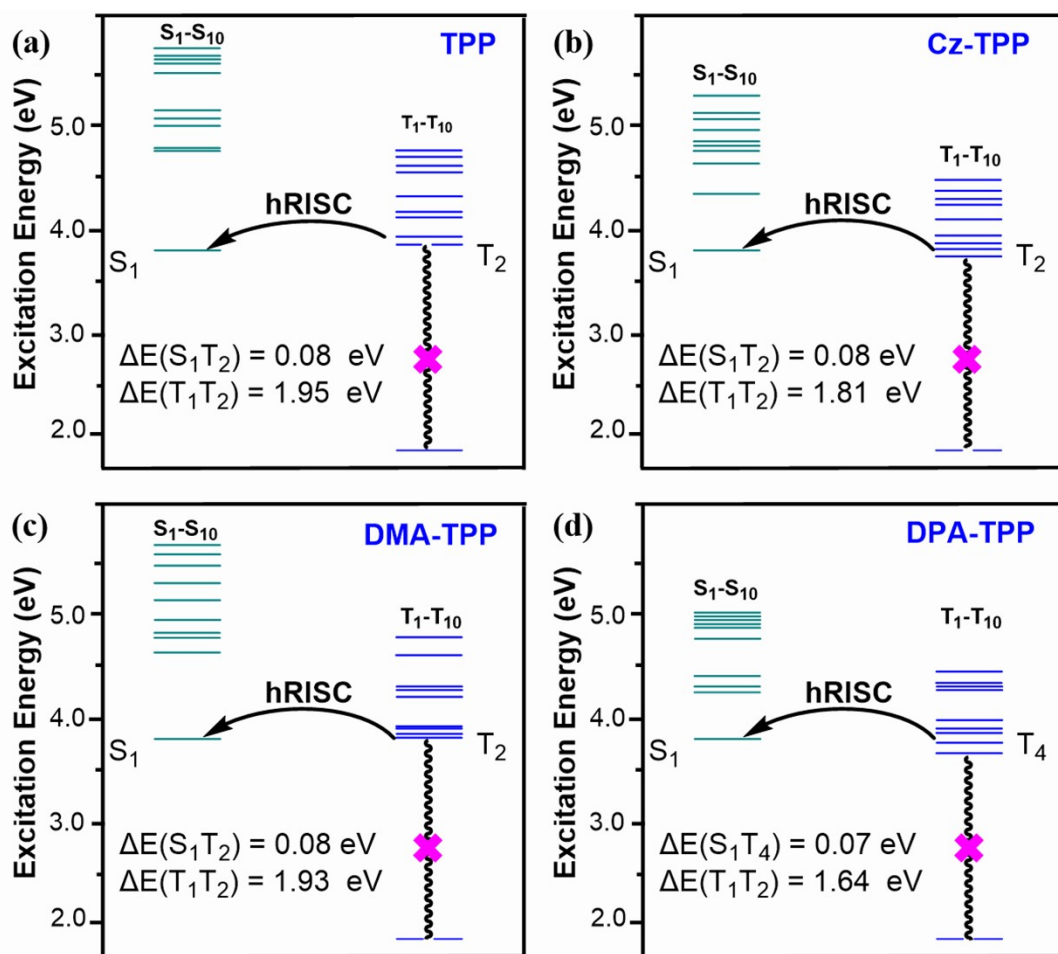


Figure S4. Energy diagram of the first ten singlet and triplet excited states for (a) TPP, (b) Cz-TPP, (c) DMA-TPP and (d) DPA-TPP from TDA-M06-2X calculations.

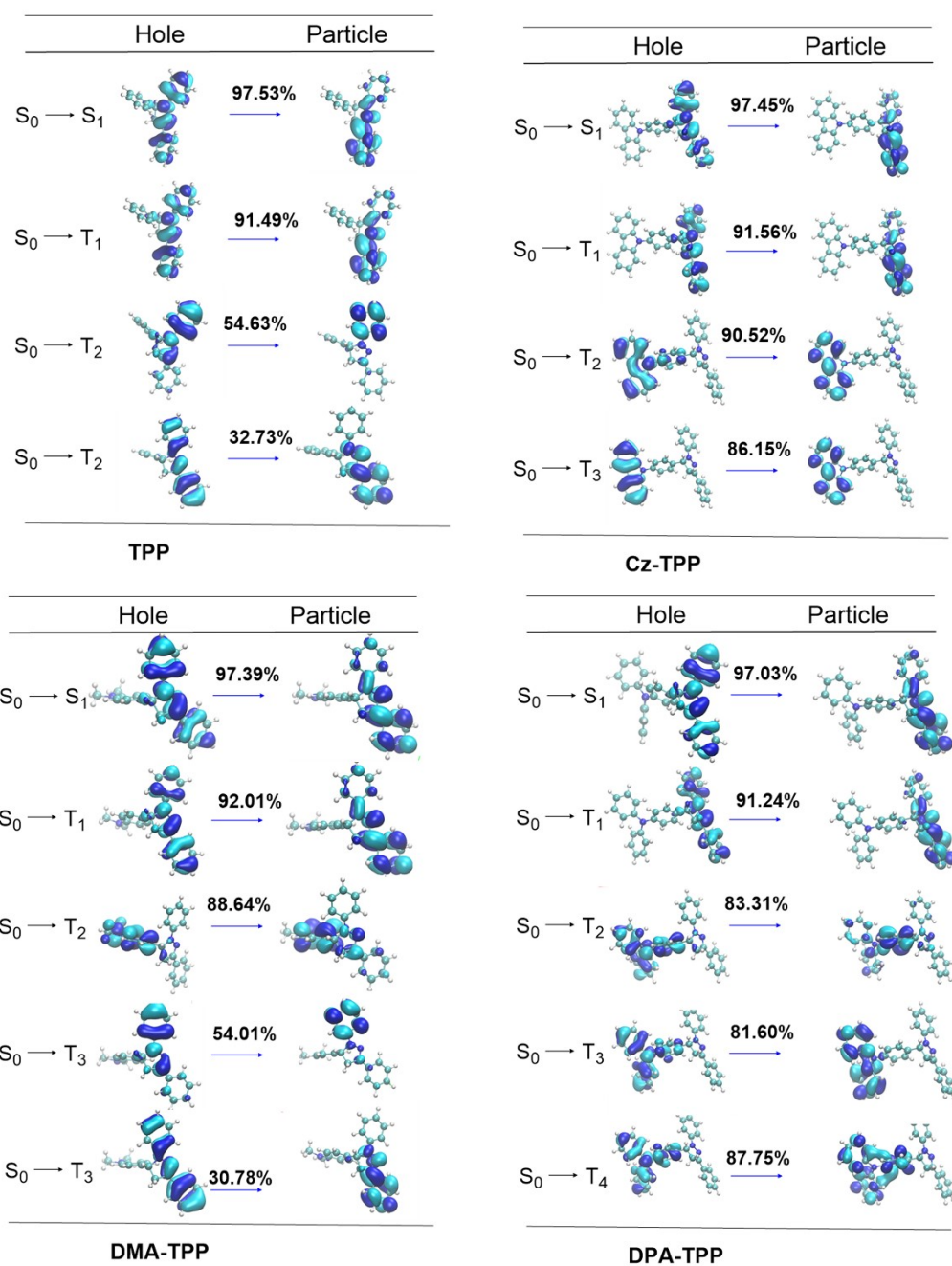


Figure S5. The NTOs distribution of **TPP**, **Cz-TPP**, **DMA-TPP** and **DPA-TPP**, respectively.

Table S1. Vertical excitation energies of **TPP** at S₁-geometry at the level of TDA-M06-2X/6-311G(d)

Excitation energy (eV)		Excitation energy (eV)	
S ₁	3.82	T ₁	1.95
S ₂	4.73	T ₂	3.90
S ₃	5.00	T ₃	3.99
S ₄	5.07	T ₄	4.29
S ₅	5.19	T ₅	4.32
S ₆	5.54	T ₆	4.49
S ₇	5.59	T ₇	4.61
S ₈	5.67	T ₈	4.69
S ₉	5.76	T ₉	4.78
S ₁₀	5.84	T ₁₀	4.85

Table S2. Vertical excitation energies of **Cz-TPP** at S₁-geometry at the level of TDA-M06-2X/6-311G(d).

Excitation energy (eV)		Excitation energy (eV)	
S ₁	3.84	T ₁	1.95
S ₂	4.35	T ₂	3.76
S ₃	4.66	T ₃	3.85
S ₄	4.78	T ₄	3.90
S ₅	4.85	T ₅	3.99
S ₆	4.86	T ₆	4.06
S ₇	4.98	T ₇	4.26
S ₈	5.02	T ₈	4.30
S ₉	5.03	T ₉	4.39
S ₁₀	5.37	T ₁₀	4.48

Table S3. Vertical excitation energies of **DMA-TPP** at S₁-geometry at the level of TDA-M06-2X/6-311G(d).

Excitation energy (eV)		Excitation energy (eV)	
S ₁	3.79	T ₁	1.94
S ₂	4.68	T ₂	3.87
S ₃	4.73	T ₃	3.90
S ₄	4.78	T ₄	3.98
S ₅	4.98	T ₅	3.99
S ₆	5.15	T ₆	4.28
S ₇	5.30	T ₇	4.32
S ₈	5.50	T ₈	4.37
S ₉	5.62	T ₉	4.62
S ₁₀	5.73	T ₁₀	4.80

Table S4. Vertical excitation energies of **DPA-TPP** at S_1 -geometry at the level of TDA-M06-2X/6-311G(d).

Excitation energy (eV)		Excitation energy (eV)	
S_1	3.81	T_1	1.96
S_2	4.27	T_2	3.60
S_3	4.30	T_3	3.75
S_4	4.43	T_4	3.88
S_5	4.70	T_5	3.90
S_6	4.89	T_6	3.99
S_7	4.90	T_7	4.28
S_8	4.92	T_8	4.31
S_9	5.00	T_9	4.33
S_{10}	5.01	T_{10}	4.48

5. Photophysical Measurements.

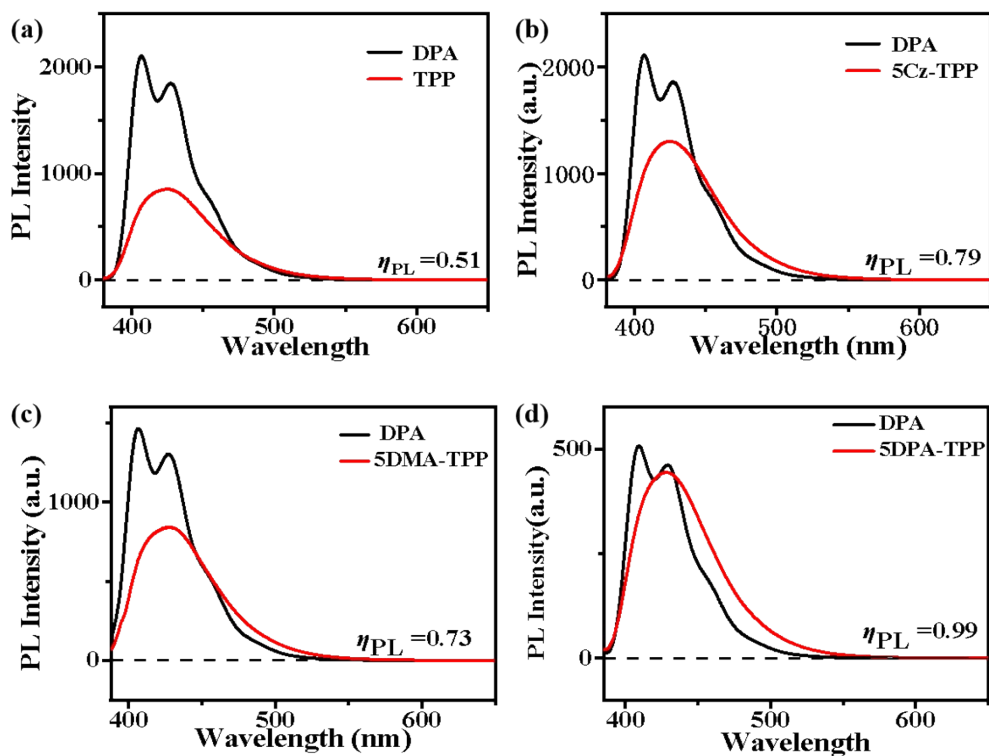


Figure S6. The relative fluorescence quantum yields (PLQY) of **TPP** derivatives in cyclohexane solution.

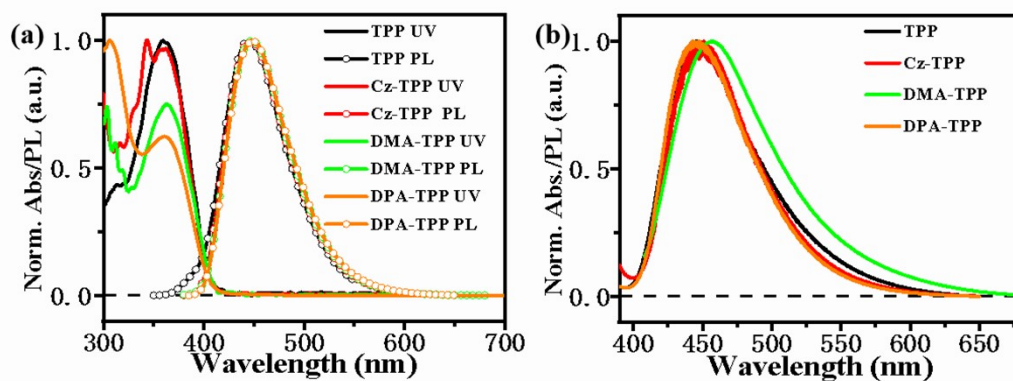


Figure S7 (a) Absorption and fluorescence spectra in dichloromethane solution. (b) Fluorescence spectra in neat films of **TPP**, **Cz-TPP**, **DMA-TPP** and **DPA-TPP**

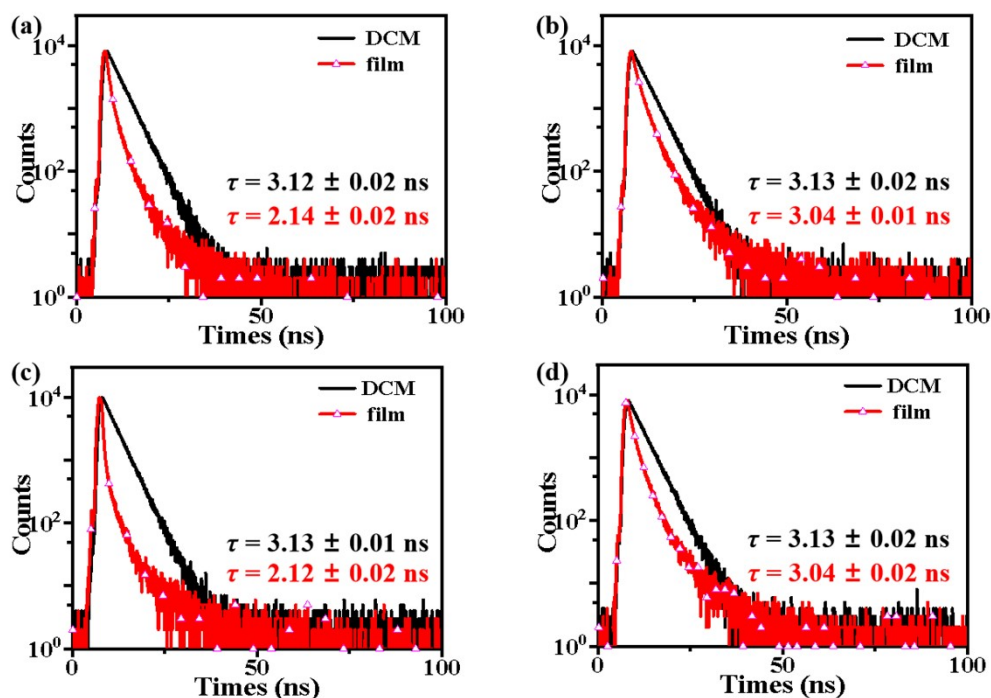


Figure S8 Transient PL decay curves in dichloromethane solution and neat film of **TPP** derivatives.

6. Single Crystal Diffraction Analysis.

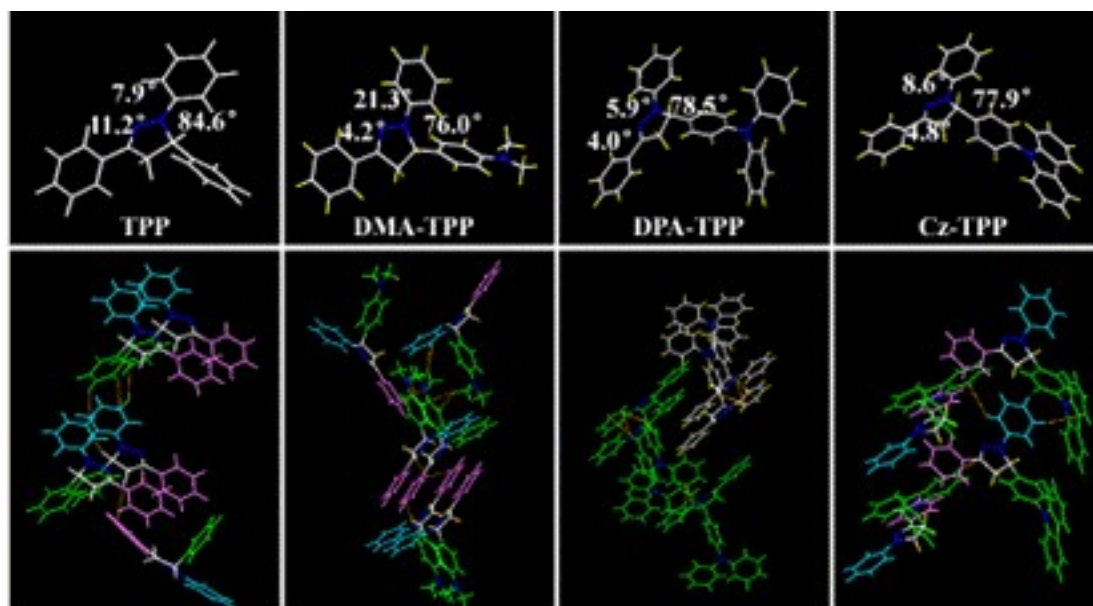


Figure S9. Crystal structure, packing pattern of TPP, DMA-TPP, DPA-TPP and Cz-TPP in crystals. The single crystals of TPP derivatives were cultivated from dichloromethane and anhydrous ethanol mixture solution by slow volatilization and then were analyzed by X-ray crystallography (CCDC: 2287503-2287505).

7. Estimation of Basic Photophysical Data.

The quantum efficiencies and rate constants were determined using the following equations according to Adachi's method (equations 1–7, 8 and 9–10).¹⁰⁻¹²

$$\Phi_{\text{prompt}} = \Phi_{\text{PL}} R_{\text{prompt}} \dots \dots \dots (1)$$

$$\Phi_{\text{delayed}} = \Phi_{\text{PL}} R_{\text{delayed}} \dots \dots \dots (2)$$

$$k_{\text{F}} = \Phi_{\text{prompt}} / \tau_{\text{prompt}} \dots \dots \dots (3)$$

$$\Phi_{\text{PL}} = k_{\text{F}} / (k_{\text{F}} + k_{\text{IC}}) \dots \dots \dots (4)$$

$$\Phi_{\text{prompt}} = k_{\text{F}} / (k_{\text{F}} + k_{\text{IC}} + k_{\text{ISC}}) \dots \dots \dots (5)$$

$$\Phi_{\text{IC}} = k_{\text{IC}} / (k_{\text{F}} + k_{\text{IC}} + k_{\text{ISC}}) \dots \dots \dots (6)$$

$$\Phi_{\text{ISC}} = k_{\text{ISC}} / (k_{\text{F}} + k_{\text{IC}} + k_{\text{ISC}}) = 1 - \Phi_{\text{prompt}} - \Phi_{\text{IC}} \dots \dots \dots (7)$$

$$\Phi_{\text{RISC}} = \Phi_{\text{delayed}} / \Phi_{\text{ISC}} \dots \dots \dots (8)$$

$$k_{\text{RISC}} = (k_{\text{p}} k_{\text{d}} \Phi_{\text{delayed}}) / (k_{\text{ISC}} \Phi_{\text{prompt}}) \dots \dots \dots (9)$$

$$k_{\text{p}} = 1 / \tau_{\text{prompt}}; k_{\text{d}} = 1 / \tau_{\text{delayed}} \dots \dots \dots (10)$$

where τ_{prompt} and τ_{delayed} represent the prompt and delayed fluorescence lifetimes, respectively, and $R_{\text{prompt}}/R_{\text{delayed}}$ mean the ratio of prompt versus delayed components.

8. Solvation Effects Measurements.

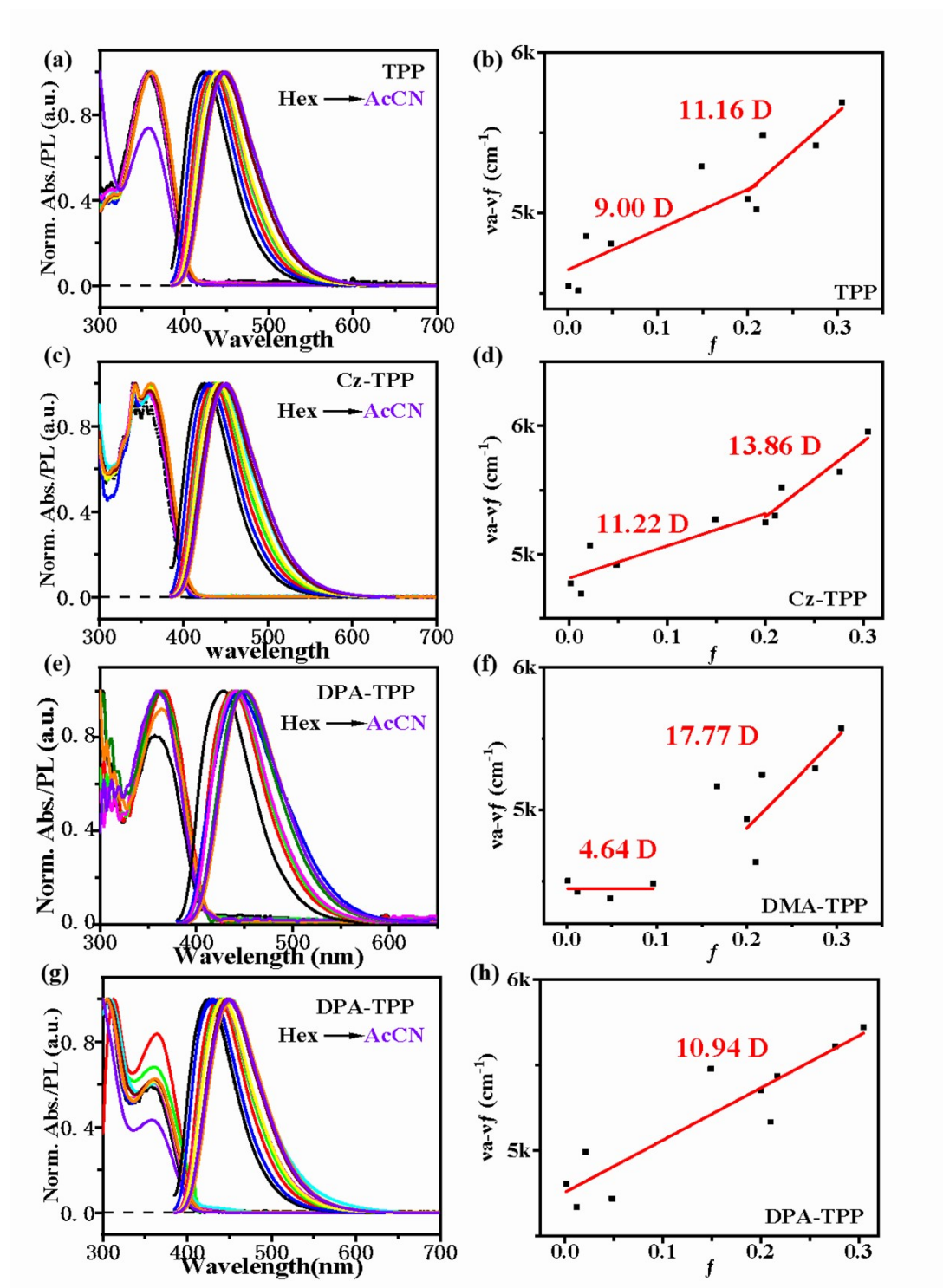


Figure S10. (a, c, e, g) Absorption and fluorescence spectra in different solvents. (b, d, f, h) The solvatochromic Lippert–Mataga models of **TPP** derivatives.

9. References.

1. A. Karuppusamy, R. Arulkumar, P. Kannan and P. Venuvanalingam, *Opt. Mate.*, 2019, **94**, 403-414.

10. Appendix.

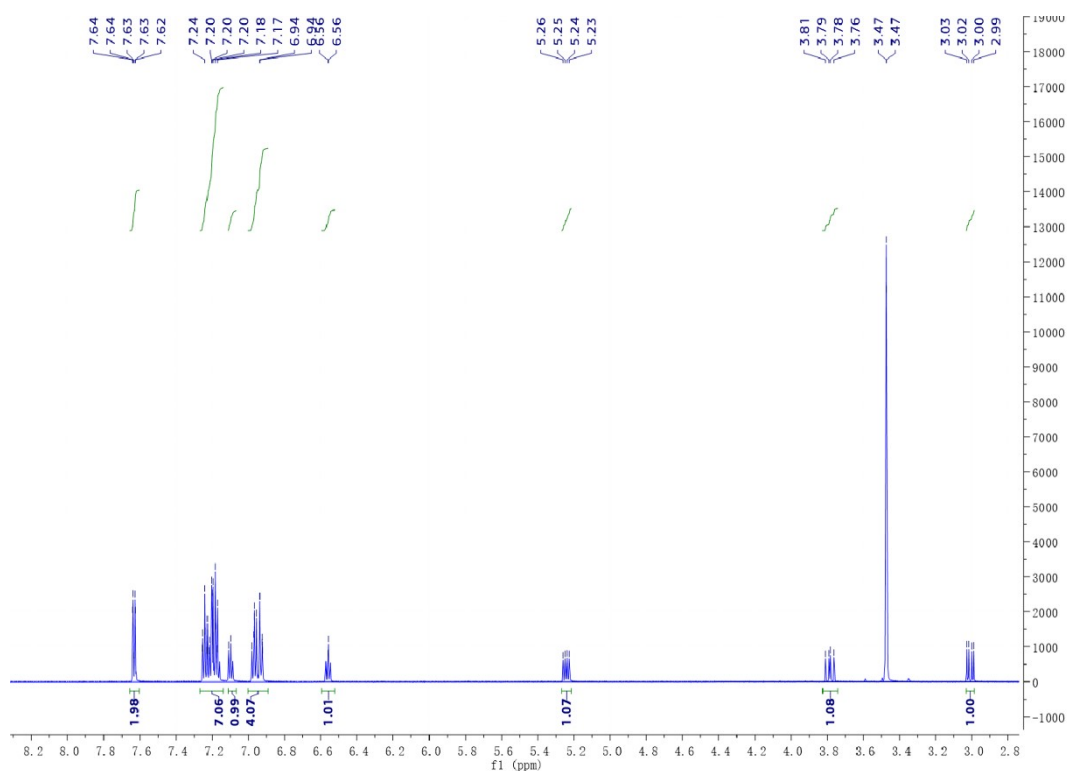


Figure S11. ¹H NMR of TPP molecule (C₄D₈O, 298 K).

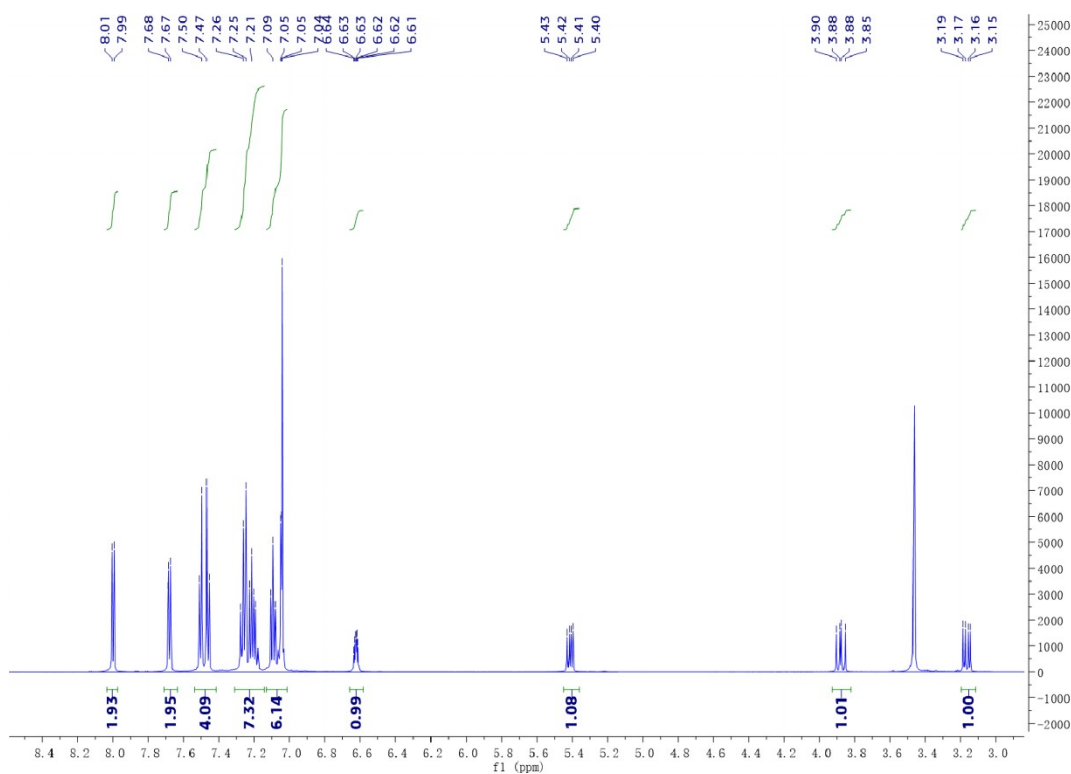


Figure S12. ¹H NMR of Cz-TPP molecule (C₄D₈O, 298 K).

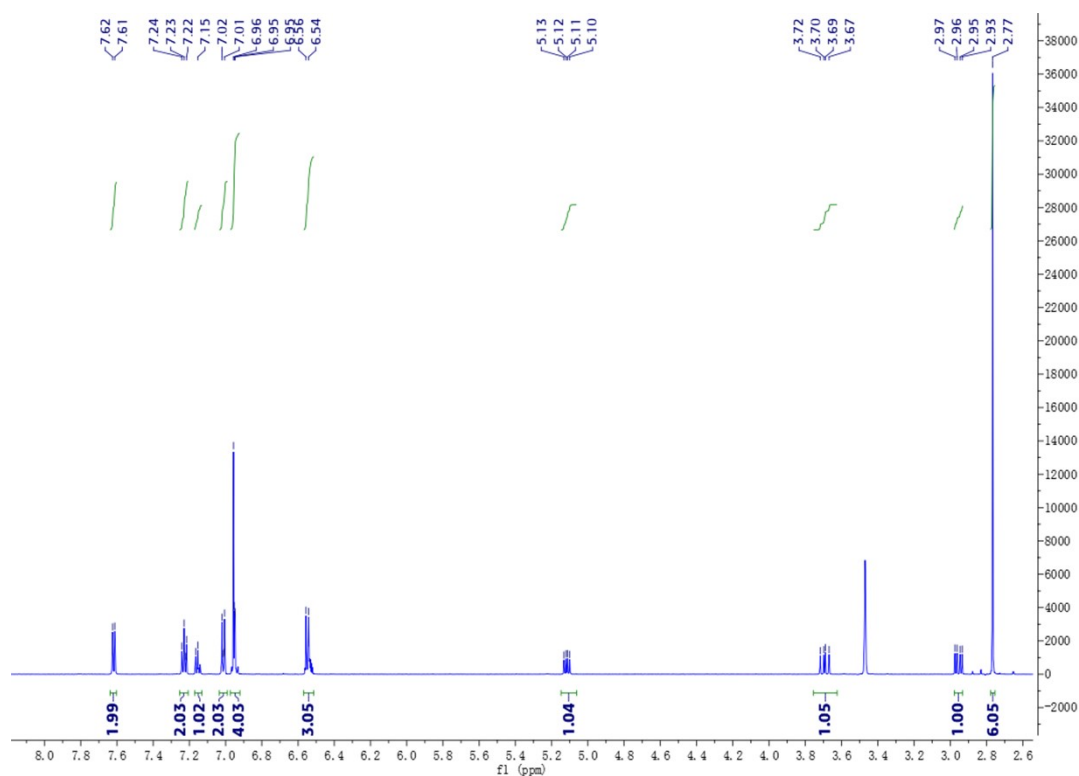


Figure S13. ¹H NMR of DMA-TPP molecule (C₄D₈O, 298 K).

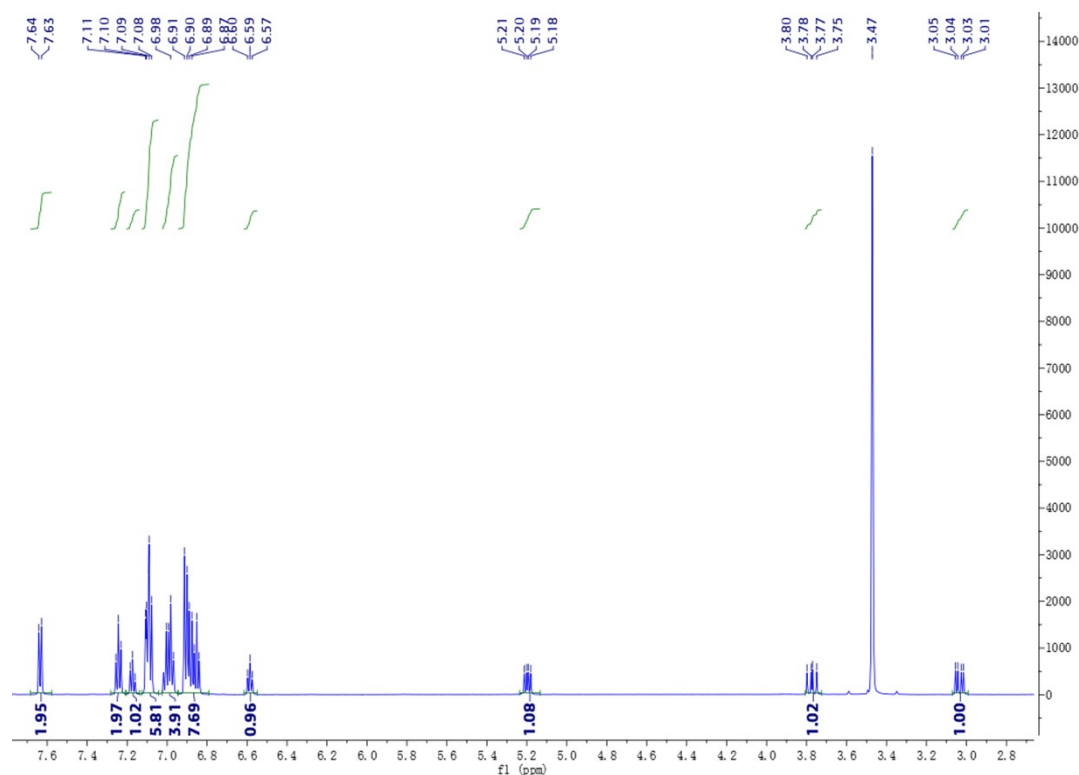


Figure S14. ¹H NMR of DPA-TPP molecule (C₄D₈O, 298 K).

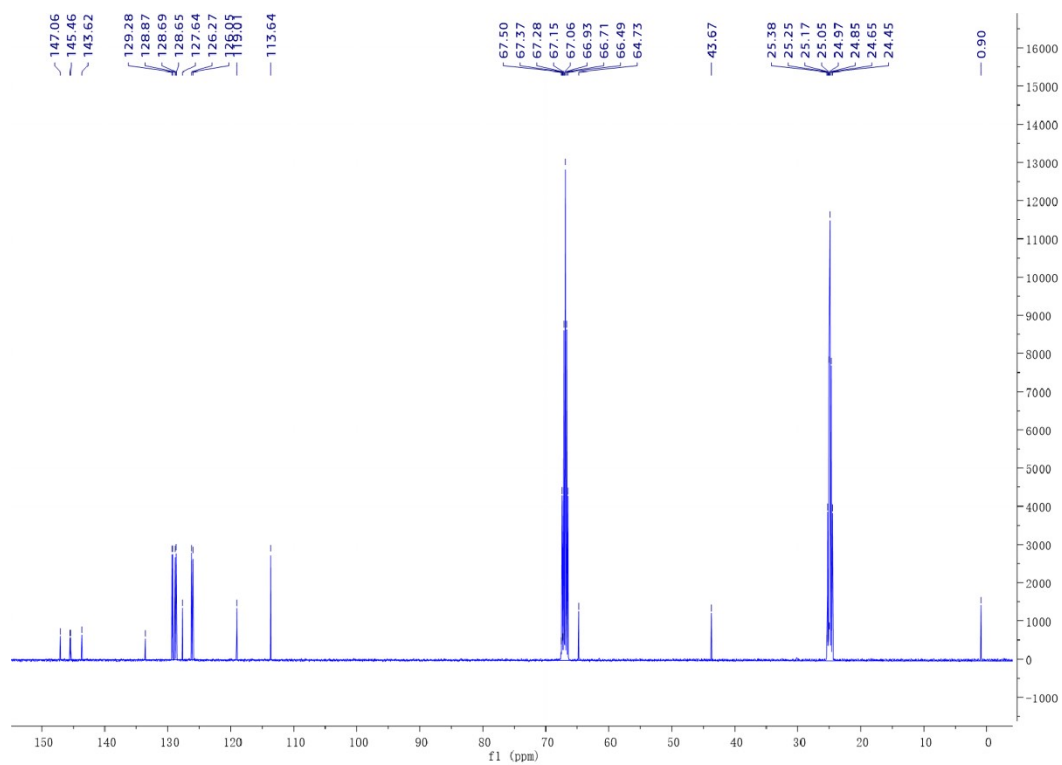


Figure S15. ¹³C NMR of **TPP** molecule (C₄D₈O, 298 K).

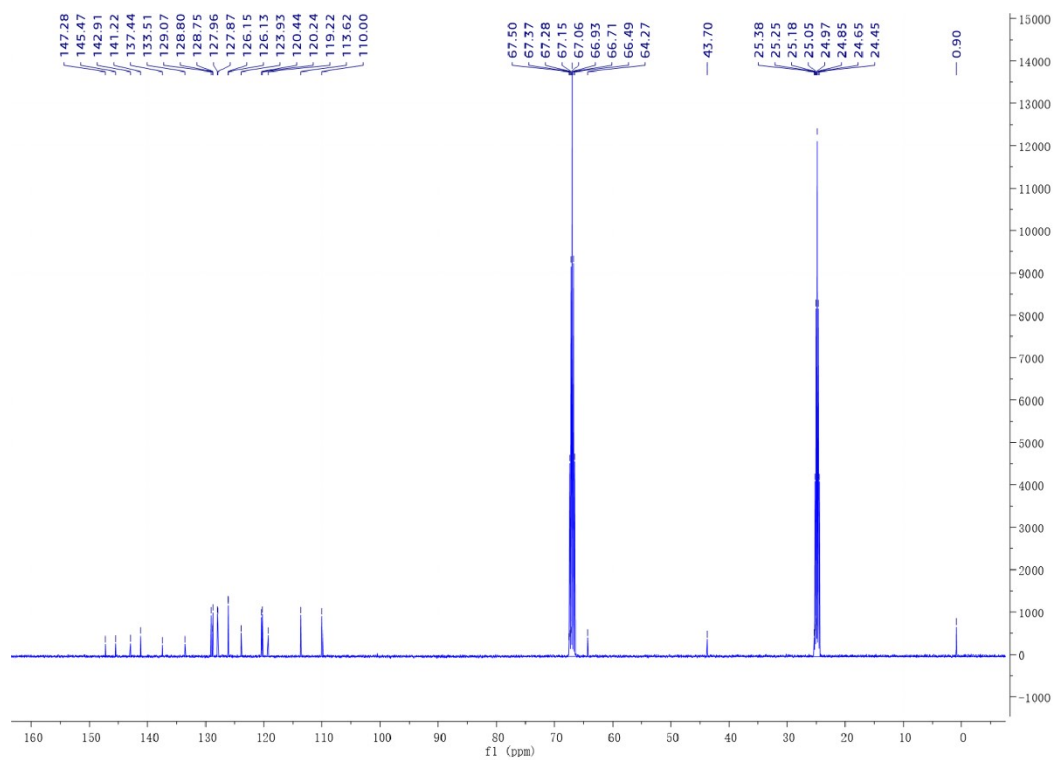


Figure S16. ¹³C NMR of **Cz-TPP** molecule (C₄D₈O, 298 K).

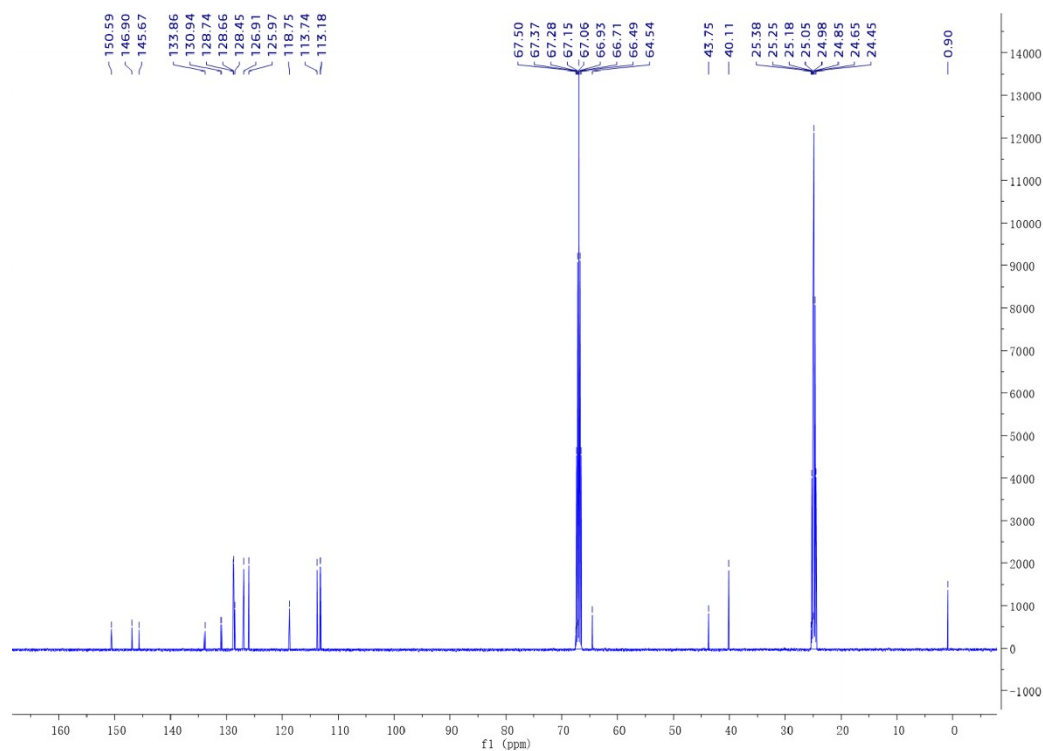


Figure S17. ¹³C NMR of **DMA-TPP** molecule (C₄D₈O, 298 K).

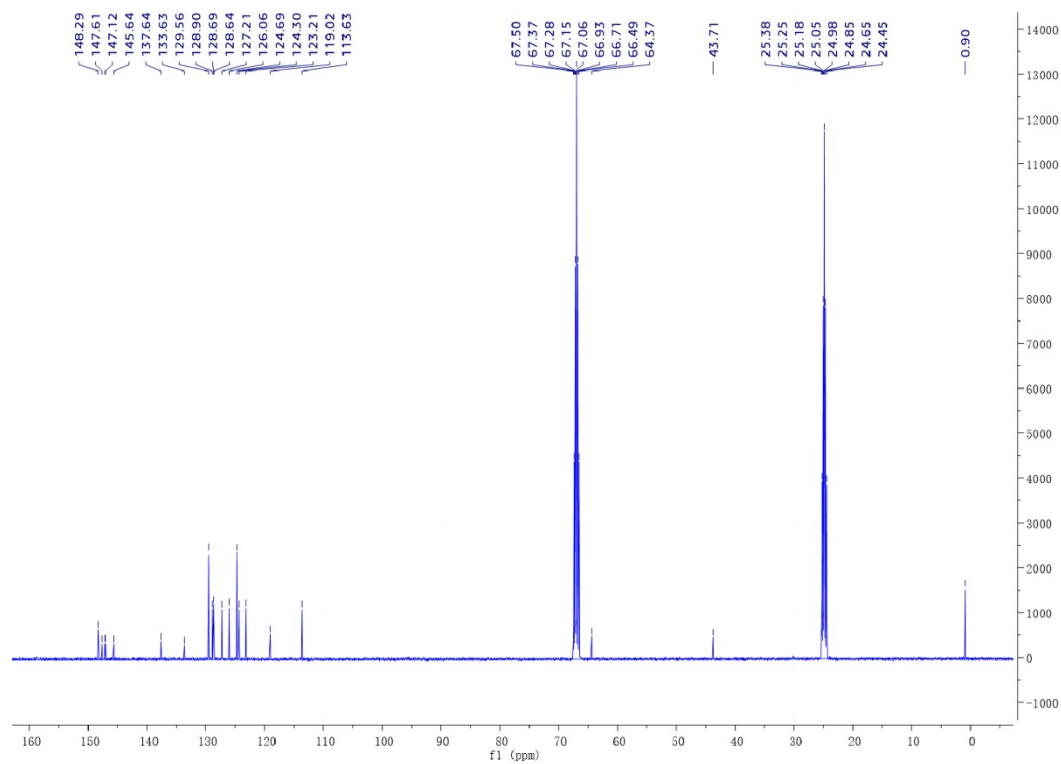


Figure S18. ¹³C NMR of **DPA-TPP** molecule (C₄D₈O, 298 K).

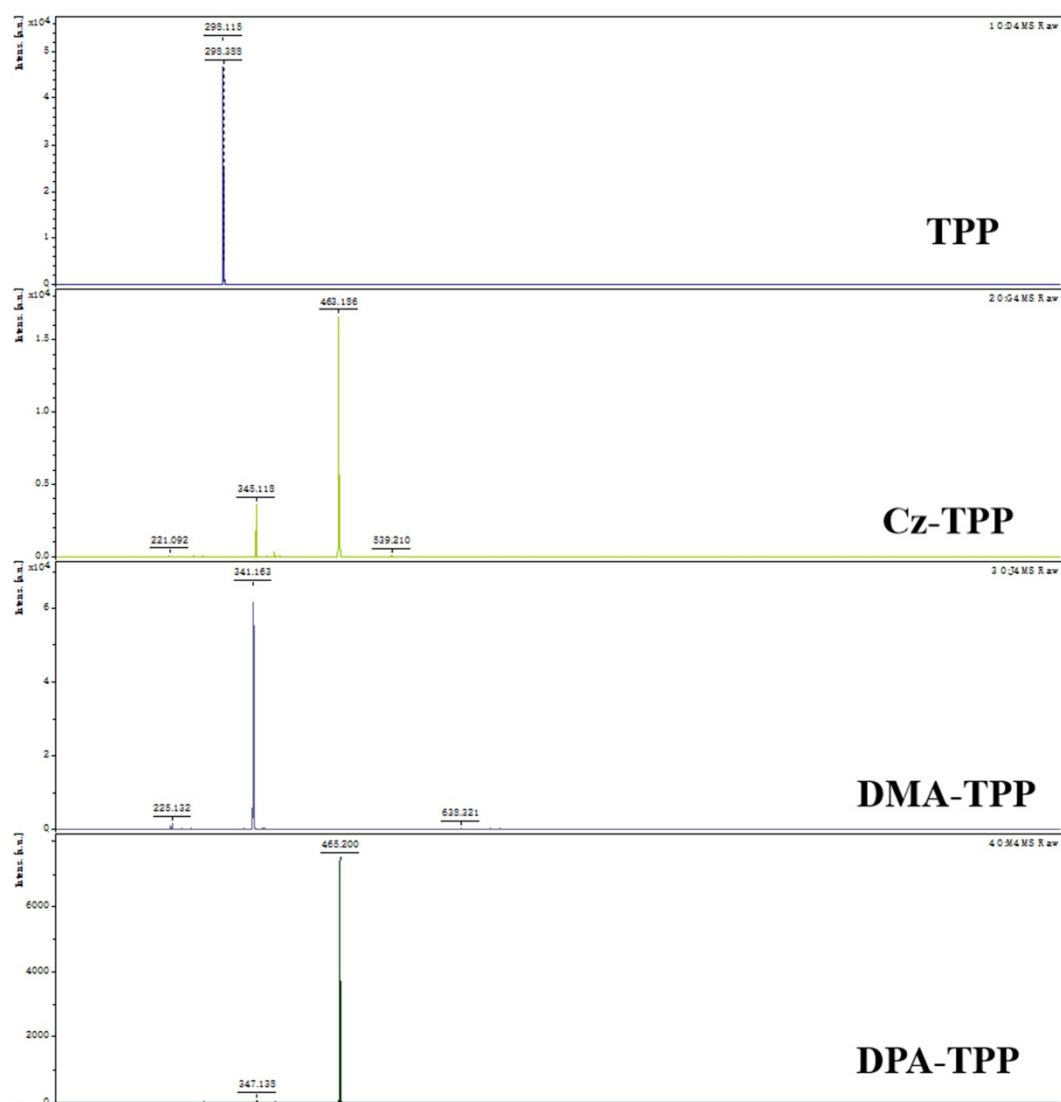


Figure S19. HMRS of **TPP** derivatives.

Cartesian coordinates for the optimized structures

Simplified TPP in Aromaticity Analysis (S_0)

C	-0.81256700	2.03627600	0.05587100
C	0.71340400	2.07416100	-0.07413800
C	1.04380600	0.59592200	-0.07044200
N	0.00570200	-0.14747200	-0.18499700
N	-1.11170400	0.63564500	-0.27022400
C	2.40078800	0.04315000	-0.00653400
C	-2.36670900	0.06485000	-0.10812100
C	3.50413000	0.89985000	0.04388000
C	4.79627600	0.38550400	0.10146600
C	5.00055000	-0.98912800	0.11081500
C	3.90413400	-1.85090300	0.06036000

C	2.61622500	-1.34204900	0.00175600
C	-3.48766900	0.88556100	0.08295900
C	-4.75217400	0.32106900	0.21229100
C	-4.92863400	-1.05664100	0.15871400
C	-3.81206300	-1.87052400	-0.02795100
C	-2.54322900	-1.32718000	-0.16067200
H	-1.14369900	2.26032400	1.07672700
H	-1.31919300	2.71090200	-0.63314200
H	1.03813100	2.52913100	-1.01441800
H	1.19081000	2.61620600	0.74192600
H	3.35812900	1.97455600	0.03386800
H	5.64241500	1.06203200	0.13892300
H	6.00637900	-1.39049400	0.15691600
H	4.05796700	-2.92404200	0.06720300
H	1.76273500	-2.00860600	-0.03761200
H	-3.37775500	1.96218300	0.12765000
H	-5.60595400	0.97349900	0.35908700
H	-5.91602500	-1.49052000	0.26108100
H	-3.92884500	-2.94804400	-0.07014100
H	-1.68068500	-1.96384900	-0.30305700

Simplified TPP in Aromaticity Analysis (T₁)

C	0.79307800	1.99849300	-0.04330400
C	-0.72448100	2.04448500	0.11395000
C	-1.10842800	0.59575400	0.06373400
N	0.02940400	-0.25879400	0.08080100
N	1.08429200	0.55867200	0.02250600
C	-2.39500100	0.07765600	0.01807600
C	2.37609800	0.04746700	0.00427100
C	-3.54521400	0.93110900	0.02353600
C	-4.81534100	0.40244200	-0.02166800
C	-5.01614800	-0.98659200	-0.07290100
C	-3.90549700	-1.83997700	-0.07593200
C	-2.62241100	-1.33589300	-0.03005400
C	3.47823700	0.90947000	-0.10535700
C	4.76269900	0.38429500	-0.11865300
C	4.97035400	-0.98948100	-0.02541400
C	3.87228000	-1.84194700	0.08068700
C	2.58109800	-1.33886000	0.09546400
H	1.13162200	2.39338700	-1.00393600
H	1.32645300	2.51677700	0.75481800
H	-1.01043000	2.50431600	1.06565600
H	-1.19739100	2.62640900	-0.68048200
H	-3.41082000	2.00678400	0.06769400

H	-5.67152200	1.06855500	-0.01623800
H	-6.01990400	-1.39277500	-0.10745600
H	-4.05491500	-2.91393600	-0.11359200
H	-1.76726000	-1.99998100	-0.03110300
H	3.33937300	1.98003800	-0.18576200
H	5.60772200	1.05752000	-0.20464400
H	5.97614700	-1.39185500	-0.03676500
H	4.02322500	-2.91299500	0.15266400
H	1.72389200	-1.99191400	0.17738100

Simplified TPP in Aromaticity Analysis (S₁)

C	-0.80485100	2.01859800	0.03111400
C	0.71879600	2.04860000	-0.03646600
C	1.07175200	0.58604500	-0.00967800
N	-0.01436900	-0.22114800	0.00295300
N	-1.10294300	0.57877100	0.00766700
C	2.37962200	0.07038100	-0.00346800
C	-2.35839200	0.06257200	0.00336800
C	3.52153600	0.92866000	-0.02361300
C	4.79740700	0.40639300	-0.01581400
C	5.00860900	-0.98225400	0.01088700
C	3.90057200	-1.84024300	0.02946000
C	2.61346000	-1.34325800	0.02218400
C	-3.49337600	0.91517500	0.02747300
C	-4.75802500	0.36538700	0.01936800
C	-4.93811700	-1.02421400	-0.01104100
C	-3.82146600	-1.86402400	-0.03178800
C	-2.54043100	-1.34777900	-0.02396700
H	-1.20303200	2.45181400	0.95162200
H	-1.28845300	2.50235500	-0.81934000
H	1.07268800	2.53594900	-0.95021800
H	1.15258000	2.59226900	0.80716300
H	3.38281700	2.00479400	-0.04668500
H	5.64862200	1.07914500	-0.03139800
H	6.01507700	-1.38407600	0.01604000
H	4.05559100	-2.91438300	0.04956000
H	1.76190200	-2.01295000	0.03639000
H	-3.37373500	1.99077900	0.05554100
H	-5.62023100	1.02171800	0.03811800
H	-5.93697800	-1.44327700	-0.01673900
H	-3.95735600	-2.93937900	-0.05378000
H	-1.67088900	-1.98834600	-0.03872700

TPP S₀ state

C	1.24560959	-1.62778383	-0.30173888
N	0.54788911	0.72930070	-0.66621482
C	0.57835301	-0.62688998	-1.22841543
C	-0.92922963	-0.90507197	-1.40316169
C	-1.53262995	0.16163679	-0.51544240
N	-0.67708299	1.04713996	-0.15487398
C	-2.94928209	0.23919149	-0.14675801
C	1.66641702	1.48631937	-0.34548625
C	1.22513754	-1.45458801	1.08147190
C	1.79716648	-2.40963857	1.91562497
C	2.39575537	-3.54423111	1.37548132
C	2.42090139	-3.72025252	-0.00468772
C	1.84844799	-2.76438726	-0.83806896
C	2.94191718	1.05994780	-0.74435849
C	4.05815432	1.83440197	-0.45222706
C	3.93611760	3.03457309	0.23984779
C	2.66855508	3.45312802	0.63861980
C	1.54099884	2.69598349	0.35487179
C	-3.41801203	1.23979668	0.71543912
C	-4.76240736	1.30611019	1.04604525
C	-5.66298186	0.37677996	0.52363743
C	-5.20636798	-0.61893366	-0.33147685
C	-3.85709815	-0.68956944	-0.66428899
H	1.09269600	-0.61797136	-2.19155921
H	-1.25627790	-0.75923722	-2.43705648
H	-1.19536215	-1.91868758	-1.10248149
H	0.77167751	-0.56482287	1.50737971
H	1.77981767	-2.26420127	2.98982626
H	2.89098566	-4.59801720	-0.43362993
H	1.87396223	-2.90081142	-1.91545619
H	3.06726863	0.12299175	-1.27311330
H	5.03493535	1.48611814	-0.76958127
H	4.81108218	3.63156605	0.46770887
H	2.55141087	4.38610968	1.17930876
H	0.55973060	3.02867571	0.66450787
H	-2.71520398	1.95869219	1.12045735
H	-5.11365472	2.08331567	1.71537739
H	-6.71358894	0.43087796	0.78518883
H	-5.89981424	-1.34443411	-0.74145716
H	-3.51305003	-1.46954438	-1.33502100
H	2.84460827	-4.28483933	2.02765093

TPP S₁ state

C	1.08683457	-1.69251723	-0.31681597
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N	0.66093734	0.72894844	-0.48795259
C	0.62758130	-0.55922738	-1.21052560
C	-0.86089520	-0.63898733	-1.58705811
C	-1.47181284	0.31486484	-0.60407929
N	-0.53952319	1.14289777	-0.04115923
C	-2.82673032	0.38711758	-0.24763421
C	1.79961122	1.42895239	-0.21209143
C	0.59113623	-1.81603314	0.98348380
C	0.98918968	-2.88269198	1.78054955
C	1.88461032	-3.83078304	1.29035887
C	2.38504592	-3.70550828	-0.00131955
C	1.98896743	-2.63770443	-0.80123419
C	3.07002227	0.94072761	-0.60342895
C	4.19932003	1.68868187	-0.33792696
C	4.10706168	2.91893760	0.32276245
C	2.85674591	3.39229950	0.72364922
C	1.70704260	2.66647086	0.47352780
C	-3.27400469	1.32609330	0.73738703
C	-4.60636846	1.38765138	1.09334833
C	-5.55215183	0.54425311	0.49909218
C	-5.13289403	-0.37618387	-0.47590607
C	-3.80917659	-0.45789832	-0.84860051
H	1.27069802	-0.48682401	-2.08815319
H	-1.00692779	-0.31072627	-2.62273070
H	-1.24667276	-1.65552857	-1.49802525
H	-0.09678682	-1.07320963	1.37657409
H	0.60101344	-2.97274315	2.78866276
H	3.08608517	-4.43647979	-0.38813555
H	2.38074626	-2.54210868	-1.80956042
H	3.16810110	-0.01964383	-1.09249299
H	5.16765474	1.30843479	-0.64163579
H	5.00139903	3.49391810	0.53052294
H	2.77995977	4.34119689	1.24233856
H	0.73528368	3.02274833	0.78301132
H	-2.54728466	1.98594747	1.19570958
H	-4.92487026	2.10445149	1.84356880
H	-6.59668829	0.60481270	0.78163845
H	-5.86036720	-1.03013943	-0.94528175
H	-3.50959745	-1.16743924	-1.61289058
H	2.19354387	-4.66068093	1.91543211

TPP T₁ state

C	0.93708000	-1.68948800	-0.32898600
N	0.71744800	0.75879700	-0.59612600

C	0.61347600	-0.54698600	-1.27085700
C	-0.86287500	-0.53273900	-1.70254900
C	-1.44772000	0.43487800	-0.72378400
N	-0.44144500	1.31389300	-0.22180000
C	-2.76326900	0.52293900	-0.28468600
C	1.93027300	1.35156700	-0.25398300
C	0.58071200	-1.62558600	1.01817200
C	0.83153400	-2.70607500	1.85745600
C	1.43910400	-3.85494600	1.35922500
C	1.79911900	-3.91998300	0.01682000
C	1.55080700	-2.83896500	-0.82323900
C	3.14472800	0.70653000	-0.53230800
C	4.34179700	1.32599400	-0.20199800
C	4.35119500	2.57722600	0.40835500
C	3.14180800	3.20917600	0.69176000
C	1.93487600	2.60843700	0.36991100
C	-3.14434000	1.48399100	0.70530300
C	-4.45021500	1.56206300	1.14424600
C	-5.43564800	0.71357500	0.62657100
C	-5.08558700	-0.22764400	-0.35390700
C	-3.78896500	-0.32822100	-0.80549900
H	1.28814600	-0.55982700	-2.12862400
H	-0.94718000	-0.16598700	-2.73227800
H	-1.30780600	-1.52653000	-1.65529400
H	0.11671800	-0.72743800	1.41545700
H	0.55470800	-2.64837800	2.90403400
H	2.27730500	-4.80976900	-0.37661200
H	1.83586500	-2.88890400	-1.87013800
H	3.16166000	-0.27649000	-0.98548200
H	5.27513200	0.81957500	-0.41904700
H	5.29011800	3.05311700	0.66463300
H	3.13736900	4.18215900	1.16974800
H	0.99174700	3.09155300	0.58328300
H	-2.38746200	2.14739000	1.10451200
H	-4.71543600	2.29488700	1.89909100
H	-6.45904900	0.78561300	0.97472200
H	-5.84516300	-0.88473900	-0.76368900
H	-3.54252000	-1.05539300	-1.57142100
H	1.63648800	-4.69411300	2.01642900

DMA-TPP S₀ state

C	1.04571270	-0.34591508	-0.90688533
N	-0.72506979	1.36841523	-0.62411055
C	-0.17073413	0.32773825	-1.50636400

C	-1.38255598	-0.61827445	-1.63680638
C	-2.26242567	-0.14597761	-0.50043335
N	-1.86227684	0.96204067	0.00888787
C	-3.48190533	-0.82738127	-0.05548278
C	-0.04232871	2.50129169	-0.20690206
C	1.15466214	-0.56083777	0.46570290
C	2.24504136	-1.22218839	1.00978977
C	3.28369696	-1.71090913	0.18959368
C	3.17733228	-1.47041821	-1.19490844
C	2.07696140	-0.80665832	-1.71981070
N	4.35964228	-2.39661995	0.72160460
C	1.18061902	2.83947186	-0.80646319
C	1.85303495	3.99120906	-0.41799953
C	1.33602599	4.82423961	0.56870773
C	0.12419061	4.48429160	1.16566524
C	-0.56480579	3.33915325	0.79077319
C	-4.26601629	-0.31099006	0.98531748
C	-5.42202434	-0.96522618	1.38216871
C	-5.81695403	-2.14515355	0.75061625
C	-5.04512159	-2.66408126	-0.28186261
C	-3.88455402	-2.00989256	-0.68300964
C	5.52904001	-2.60129472	-0.11323270
C	4.55591210	-2.36881025	2.15927855
H	0.08971663	0.76604896	-2.47257019
H	-1.90396663	-0.49315542	-2.59051286
H	-1.08803224	-1.66413381	-1.54675929
H	0.38138089	-0.18865989	1.13208318
H	2.28727160	-1.34966323	2.08305703
H	3.95679270	-1.79412412	-1.87131249
H	2.03120555	-0.63678324	-2.79232209
H	1.61056691	2.20176547	-1.56852139
H	2.79634862	4.23322328	-0.89535384
H	1.86687176	5.72010692	0.86783567
H	-0.29600494	5.12011607	1.93756785
H	-1.50690682	3.08374686	1.25673018
H	-3.95680282	0.60568349	1.47400457
H	-6.02104441	-0.55595432	2.18785872
H	-6.72133118	-2.65412251	1.06386939
H	-5.34432381	-3.57961577	-0.77932148
H	-3.29295937	-2.42303324	-1.49252376
H	5.28655742	-3.22270925	-0.97806797
H	5.95433559	-1.65672766	-0.47759487
H	6.28989482	-3.12438147	0.46174447
H	4.67076885	-1.34867213	2.54879573

H	3.71649782	-2.83974626	2.67526568
H	5.45027150	-2.93637945	2.40665746

DMA-TPP S₁ state

C	1.05804996	-0.18739134	-0.90488224
N	-0.71828936	1.46776901	-0.48607147
C	-0.11446098	0.56634830	-1.49054244
C	-1.32018663	-0.32907179	-1.82656336
C	-2.18286715	-0.13637446	-0.61488484
N	-1.83414519	0.98294192	0.08972068
C	-3.22421758	-0.97292598	-0.18732679
C	-0.17718162	2.65341230	-0.08295539
C	1.00056733	-0.72549550	0.38160250
C	2.05152187	-1.46574388	0.89783038
C	3.21363900	-1.71302303	0.13543671
C	3.27263573	-1.14266183	-1.15277145
C	2.21283954	-0.39912027	-1.65231900
N	4.24774196	-2.47918630	0.63056523
C	1.05088323	3.11828853	-0.61475223
C	1.55318264	4.33622627	-0.20198310
C	0.87132069	5.11333967	0.74154664
C	-0.33031941	4.64716171	1.27763249
C	-0.85869840	3.43133905	0.88674989
C	-3.94579367	-0.68554659	1.01693532
C	-4.95806428	-1.52112761	1.44481088
C	-5.31161256	-2.66127862	0.71333492
C	-4.62249272	-2.95223781	-0.47623082
C	-3.60845525	-2.13466227	-0.92486816
C	5.51077932	-2.49043222	-0.08364052
C	4.26057498	-2.80282388	2.04550708
H	0.20544982	1.16157277	-2.34705570
H	-1.81481830	0.02409130	-2.73940318
H	-1.01935154	-1.36542985	-1.98425210
H	0.12705415	-0.55014319	1.00371702
H	1.96361330	-1.85030864	1.90478420
H	4.14952043	-1.27235662	-1.77229046
H	2.29431573	0.02314170	-2.65010107
H	1.60677313	2.52086593	-1.32605585
H	2.49361414	4.68625436	-0.61189250
H	1.27898434	6.06509598	1.06053418
H	-0.85937335	5.24088790	2.01442693
H	-1.78668976	3.05983761	1.29663721
H	-3.68091106	0.19771824	1.58555081
H	-5.48983427	-1.28637514	2.36144262

H	-6.11177328	-3.30730132	1.05513389
H	-4.89383604	-3.83035884	-1.05304365
H	-3.09700325	-2.37330491	-1.85148208
H	5.38751140	-2.90660085	-1.08610031
H	5.94731261	-1.48773985	-0.17885702
H	6.21491358	-3.12470720	0.44986275
H	4.26507907	-1.90639854	2.67885414
H	3.39264995	-3.40842630	2.31529569
H	5.14978346	-3.38787962	2.26879439

DMA-TPP T₁ state

C	1.00238900	-0.16822800	-0.93314900
N	-0.72588700	1.55161900	-0.53029400
C	-0.12739200	0.64193800	-1.52813500
C	-1.35387500	-0.20845600	-1.90556200
C	-2.20535200	-0.05907600	-0.68527100
N	-1.87982200	1.14298100	0.00924600
C	-3.18092300	-0.92416500	-0.20370900
C	-0.11210100	2.71707600	-0.08083100
C	0.92531200	-0.67144100	0.36524400
C	1.93405200	-1.46263400	0.89175500
C	3.07234000	-1.79687400	0.12737300
C	3.15128500	-1.26691900	-1.17674300
C	2.13254100	-0.47411000	-1.68607300
N	4.06636100	-2.60755100	0.63658900
C	1.15635400	3.08802400	-0.55254300
C	1.73606700	4.26718100	-0.10589100
C	1.07665000	5.08340300	0.80947100
C	-0.17902000	4.70580400	1.28178400
C	-0.77618400	3.53274000	0.84854900
C	-3.87533000	-0.64352000	1.01611900
C	-4.83985600	-1.50834900	1.49200500
C	-5.16972100	-2.67453400	0.79171000
C	-4.50785300	-2.96306500	-0.41204600
C	-3.54009500	-2.11775200	-0.90622300
C	5.32553100	-2.69559300	-0.07952400
C	4.07409500	-2.88481100	2.06154400
H	0.23257600	1.23215900	-2.37320500
H	-1.84513600	0.21469600	-2.79011800
H	-1.07818500	-1.23927500	-2.12644100
H	0.06897800	-0.42911500	0.98918900
H	1.83257900	-1.81758900	1.90825300
H	4.01185900	-1.46728900	-1.80064000
H	2.22819500	-0.08267500	-2.69526700

H	1.69617600	2.45616600	-1.24607200
H	2.71679400	4.54565400	-0.47394600
H	1.53746500	6.00140400	1.15433400
H	-0.70073500	5.33217100	1.99639300
H	-1.75070500	3.23228400	1.20631100
H	-3.62810200	0.26023800	1.55885900
H	-5.35119500	-1.27758000	2.42065500
H	-5.93050500	-3.34583400	1.17175300
H	-4.76240200	-3.86244300	-0.96253700
H	-3.04689800	-2.35420600	-1.84260700
H	5.18039100	-3.12986200	-1.07122800
H	5.80789300	-1.71674800	-0.20015000
H	6.00086800	-3.34885100	0.46828300
H	4.12488400	-1.96927900	2.66508200
H	3.18065900	-3.43972300	2.35608500
H	4.93650100	-3.50348200	2.29909700

DPA-TPP S₀ state

C	-0.65017908	0.68426683	-1.08651988
N	-2.81882396	1.61899726	-0.32805778
C	-2.05356382	1.10723277	-1.47452353
C	-2.93889638	-0.08208390	-1.90786890
C	-3.80129186	-0.27554066	-0.67982294
N	-3.70853623	0.70082355	0.14725165
C	-4.70526654	-1.40691004	-0.45025540
C	-2.45939159	2.71597688	0.44400375
C	-0.38625396	0.12906077	0.16559757
C	0.89342222	-0.28740037	0.50206220
C	1.94099727	-0.16652717	-0.41635244
C	1.67971545	0.38376129	-1.67299063
C	0.39778125	0.81040829	-1.99556710
N	3.24775514	-0.58982620	-0.07195563
C	-1.44139742	3.57791426	0.01033077
C	-1.10465696	4.69426431	0.76651637
C	-1.76128901	4.97548883	1.95983486
C	-2.77006979	4.11618704	2.38943267
C	-3.12220549	2.99697386	1.64851982
C	-5.43124160	-1.51126023	0.74429505
C	-6.29170513	-2.57726697	0.95123148
C	-6.44381533	-3.55939927	-0.02840285
C	-5.72741459	-3.46424096	-1.21546652
C	-4.86104698	-2.39542702	-1.42621561
C	4.36371217	0.20390396	-0.42806158
C	3.42666016	-1.81215258	0.62056663

H	-2.00481836	1.86700455	-2.25715599
H	-3.56502595	0.16792220	-2.76954104
H	-2.34606757	-0.96082345	-2.16298462
H	-1.18318198	0.04357927	0.89824014
H	1.09032087	-0.70449914	1.48340738
H	2.48540520	0.48494376	-2.39150142
H	0.21278356	1.24383903	-2.97424333
H	-0.90859048	3.37794862	-0.91111505
H	-0.31480772	5.34821792	0.41346860
H	-1.49229672	5.84671676	2.54513316
H	-3.29423071	4.31725923	3.31750703
H	-3.90831611	2.33569450	1.98674564
H	-5.30920465	-0.74782689	1.50367251
H	-6.84701331	-2.64692097	1.87979011
H	-7.11806933	-4.39196002	0.13643647
H	-5.84161956	-4.22246475	-1.98187313
H	-4.31013253	-2.33047075	-2.35847089
C	5.55693564	-0.39343935	-0.84664860
C	6.65013477	0.39300782	-1.18885477
C	6.56839027	1.78159327	-1.13739970
C	4.37792529	-1.92050638	1.63953984
C	4.54865501	-3.12510581	2.31041385
C	3.76565903	-4.23109001	1.99067945
C	2.81201023	-4.12138997	0.98276515
C	2.64629856	-2.92581034	0.29495022
H	4.97984642	-1.05764809	1.90223746
H	5.29051905	-3.19459845	3.09819088
H	3.89733398	-5.16729444	2.52011260
H	2.19899344	-4.97590530	0.71853948
H	1.91025512	-2.84673879	-0.49736392
C	5.37842373	2.37742809	-0.72932380
C	4.28569206	1.59921120	-0.36826897
H	5.62264628	-1.47419760	-0.90186661
H	7.56813775	-0.08602318	-1.51078829
H	7.42135949	2.39117102	-1.41169761
H	5.30069019	3.45776444	-0.67722261
H	3.36595352	2.06857785	-0.03750334

DPA-TPP S₁ state

C	-0.65017908	0.68426683	-1.08651988
N	-2.81882396	1.61899726	-0.32805778
C	-2.05356382	1.10723277	-1.47452353
C	-2.93889638	-0.08208390	-1.90786890
C	-3.80129186	-0.27554066	-0.67982294

N	-3.70853623	0.70082355	0.14725165
C	-4.70526654	-1.40691004	-0.45025540
C	-2.45939159	2.71597688	0.44400375
C	-0.38625396	0.12906077	0.16559757
C	0.89342222	-0.28740037	0.50206220
C	1.94099727	-0.16652717	-0.41635244
C	1.67971545	0.38376129	-1.67299063
C	0.39778125	0.81040829	-1.99556710
N	3.24775514	-0.58982620	-0.07195563
C	-1.44139742	3.57791426	0.01033077
C	-1.10465696	4.69426431	0.76651637
C	-1.76128901	4.97548883	1.95983486
C	-2.77006979	4.11618704	2.38943267
C	-3.12220549	2.99697386	1.64851982
C	-5.43124160	-1.51126023	0.74429505
C	-6.29170513	-2.57726697	0.95123148
C	-6.44381533	-3.55939927	-0.02840285
C	-5.72741459	-3.46424096	-1.21546652
C	-4.86104698	-2.39542702	-1.42621561
C	4.36371217	0.20390396	-0.42806158
C	3.42666016	-1.81215258	0.62056663
H	-2.00481836	1.86700455	-2.25715599
H	-3.56502595	0.16792220	-2.76954104
H	-2.34606757	-0.96082345	-2.16298462
H	-1.18318198	0.04357927	0.89824014
H	1.09032087	-0.70449914	1.48340738
H	2.48540520	0.48494376	-2.39150142
H	0.21278356	1.24383903	-2.97424333
H	-0.90859048	3.37794862	-0.91111505
H	-0.31480772	5.34821792	0.41346860
H	-1.49229672	5.84671676	2.54513316
H	-3.29423071	4.31725923	3.31750703
H	-3.90831611	2.33569450	1.98674564
H	-5.30920465	-0.74782689	1.50367251
H	-6.84701331	-2.64692097	1.87979011
H	-7.11806933	-4.39196002	0.13643647
H	-5.84161956	-4.22246475	-1.98187313
H	-4.31013253	-2.33047075	-2.35847089
C	5.55693564	-0.39343935	-0.84664860
C	6.65013477	0.39300782	-1.18885477
C	6.56839027	1.78159327	-1.13739970
C	4.37792529	-1.92050638	1.63953984
C	4.54865501	-3.12510581	2.31041385
C	3.76565903	-4.23109001	1.99067945

C	2.81201023	-4.12138997	0.98276515
C	2.64629856	-2.92581034	0.29495022
H	4.97984642	-1.05764809	1.90223746
H	5.29051905	-3.19459845	3.09819088
H	3.89733398	-5.16729444	2.52011260
H	2.19899344	-4.97590530	0.71853948
H	1.91025512	-2.84673879	-0.49736392
C	5.37842373	2.37742809	-0.72932380
C	4.28569206	1.59921120	-0.36826897
H	5.62264628	-1.47419760	-0.90186661
H	7.56813775	-0.08602318	-1.51078829
H	7.42135949	2.39117102	-1.41169761
H	5.30069019	3.45776444	-0.67722261
H	3.36595352	2.06857785	-0.03750334

DPA-TPP T₁ state

C	-0.74770200	0.71452700	-1.10810500
N	-2.91856300	1.56045500	-0.29905000
C	-2.15278300	1.13239800	-1.48565100
C	-3.02274200	-0.03224200	-1.98709800
C	-3.75830200	-0.41680100	-0.74297300
N	-3.79376200	0.67006900	0.18112400
C	-4.34225000	-1.63904300	-0.43318700
C	-2.67639900	2.75198400	0.38015000
C	-0.50718700	-0.01531900	0.05641500
C	0.77821200	-0.41916900	0.38559800
C	1.85514100	-0.11072000	-0.45287500
C	1.61454400	0.61506500	-1.62262400
C	0.32710500	1.02880000	-1.93688100
N	3.16786800	-0.51338800	-0.11748600
C	-1.68627900	3.63994200	-0.06713300
C	-1.46930500	4.82801000	0.61558600
C	-2.21968700	5.14770800	1.74410400
C	-3.19812300	4.26037700	2.18814500
C	-3.43179900	3.06824400	1.52011600
C	-4.97754200	-1.84675600	0.83277500
C	-5.55434700	-3.06206100	1.13984600
C	-5.54151400	-4.11723200	0.22081000
C	-4.93200200	-3.93149900	-1.03032900
C	-4.34696500	-2.72954900	-1.35963300
C	4.25238700	0.37641100	-0.31883000
C	3.38950600	-1.77348000	0.49040200
H	-2.12171100	1.95360100	-2.20377300
H	-3.70836300	0.32144600	-2.76633800

H	-2.41882700	-0.83770100	-2.40493300
H	-1.32668200	-0.24671500	0.73090100
H	0.95580400	-0.96918800	1.30260000
H	2.44124200	0.86097400	-2.27934000
H	0.15847400	1.59600600	-2.84762200
H	-1.07665500	3.40453000	-0.92972500
H	-0.70138300	5.50654400	0.26251000
H	-2.04167700	6.07622600	2.27314200
H	-3.78677900	4.49877800	3.06678200
H	-4.18852300	2.37449600	1.85868900
H	-4.99558100	-1.03163200	1.54510900
H	-6.02668000	-3.19835300	2.10710200
H	-6.00173200	-5.06625300	0.46849000
H	-4.92381500	-4.74387800	-1.74910700
H	-3.89154300	-2.60343000	-2.33600600
C	5.48115500	-0.10328600	-0.78182100
C	6.54677100	0.76877100	-0.96605200
C	6.39988100	2.12939300	-0.70989800
C	4.31054900	-1.90696800	1.53362000
C	4.52508200	-3.14750900	2.12186800
C	3.81604500	-4.26591500	1.69355300
C	2.89313500	-4.13226500	0.65989800
C	2.68507600	-2.89962300	0.05396600
H	4.85585900	-1.03594500	1.87926600
H	5.24323500	-3.23546600	2.92941800
H	3.97987400	-5.23055900	2.15944400
H	2.33710800	-4.99595400	0.31264300
H	1.97328700	-2.80212100	-0.75810200
C	5.17403600	2.60890400	-0.25718700
C	4.10805300	1.74120200	-0.05345900
H	5.59509600	-1.16078500	-0.99271100
H	7.49413500	0.38218900	-1.32504300
H	7.23069100	2.80844300	-0.86080300
H	5.04706500	3.66492400	-0.04659500
H	3.15879000	2.11607200	0.31319700

Cz-TPP S₀ state

C	0.80570357	0.67547131	1.12235514
N	3.02082548	1.51328992	0.37483181
C	2.23816547	1.00187335	1.50643711
C	3.04543600	-0.26200755	1.87096527
C	3.84789540	-0.47233477	0.60531902
N	3.81521583	0.54626512	-0.17363217
C	4.63983081	-1.66728388	0.29848910

C	2.72180536	2.66580606	-0.34236997
C	-0.19734847	0.72701300	2.08842603
C	-1.50287203	0.36800901	1.77758147
C	-1.81843155	-0.02957544	0.48031278
C	-0.82532514	-0.06979884	-0.49693427
C	0.48030639	0.27356338	-0.17254457
N	-3.14933760	-0.39013902	0.15215137
C	1.76268958	3.56699743	0.14209135
C	1.48689698	4.73416603	-0.55999732
C	2.14721234	5.02764024	-1.74817252
C	3.09777639	4.12920719	-2.22793395
C	3.38906752	2.95932736	-1.54097146
C	4.74109510	-2.70232043	1.23207652
C	5.49824348	-3.83565408	0.94996774
C	6.15914120	-3.94833335	-0.26741016
C	6.06120547	-2.91965243	-1.20490914
C	5.30941886	-1.78922169	-0.92688529
C	-3.54373594	-1.59497165	-0.42098063
C	-4.27969472	0.39454369	0.35778910
H	2.24544154	1.72522347	2.32380303
H	3.71932346	-0.08558217	2.71468914
H	2.39951701	-1.10372373	2.12096417
H	0.04395590	1.04214105	3.09902895
H	-2.27886473	0.39120177	2.53465909
H	-1.08444722	-0.35742206	-1.50975342
H	1.24588053	0.24810961	-0.94141803
H	1.22616199	3.35777320	1.05953468
H	0.74150227	5.41807387	-0.16904453
H	1.92506232	5.93811985	-2.29157405
H	3.62388705	4.33960816	-3.15277176
H	4.12975027	2.26690597	-1.91762410
H	4.23299112	-2.62450586	2.18732494
H	5.57103234	-4.62970894	1.68434171
H	6.74669353	-4.83179949	-0.48958901
H	6.57276572	-3.00403219	-2.15708642
H	5.22806211	-0.99006881	-1.65425245
C	-4.94498524	-1.58773073	-0.58724010
C	-5.58186534	-2.70220723	-1.13662870
C	-4.81753924	-3.79951028	-1.50304184
C	-5.41671209	-0.31265807	-0.08819262
C	-6.67794605	0.27945147	-0.00034031
C	-6.78360650	1.55993041	0.52105475
C	-5.64128094	2.25428522	0.94715245
C	-4.37705899	1.68813077	0.87245348

H	-7.56002070	-0.25402924	-0.33839262
H	-7.75541067	2.03328439	0.59821265
H	-5.74632437	3.25795143	1.34337296
H	-3.49872176	2.23574673	1.19325763
C	-3.42663805	-3.79532682	-1.31789674
C	-2.76947957	-2.70057522	-0.77575401
H	-6.65822335	-2.70875295	-1.27148649
H	-5.29571888	-4.67154550	-1.93321525
H	-2.84943211	-4.66772960	-1.60301307
H	-1.69600987	-2.70867187	-0.62903139

Cz-TPP S₁ state

C	0.80570357	0.67547131	1.12235514
N	3.02082548	1.51328992	0.37483181
C	2.23816547	1.00187335	1.50643711
C	3.04543600	-0.26200755	1.87096527
C	3.84789540	-0.47233477	0.60531902
N	3.81521583	0.54626512	-0.17363217
C	4.63983081	-1.66728388	0.29848910
C	2.72180536	2.66580606	-0.34236997
C	-0.19734847	0.72701300	2.08842603
C	-1.50287203	0.36800901	1.77758147
C	-1.81843155	-0.02957544	0.48031278
C	-0.82532514	-0.06979884	-0.49693427
C	0.48030639	0.27356338	-0.17254457
N	-3.14933760	-0.39013902	0.15215137
C	1.76268958	3.56699743	0.14209135
C	1.48689698	4.73416603	-0.55999732
C	2.14721234	5.02764024	-1.74817252
C	3.09777639	4.12920719	-2.22793395
C	3.38906752	2.95932736	-1.54097146
C	4.74109510	-2.70232043	1.23207652
C	5.49824348	-3.83565408	0.94996774
C	6.15914120	-3.94833335	-0.26741016
C	6.06120547	-2.91965243	-1.20490914
C	5.30941886	-1.78922169	-0.92688529
C	-3.54373594	-1.59497165	-0.42098063
C	-4.27969472	0.39454369	0.35778910
H	2.24544154	1.72522347	2.32380303
H	3.71932346	-0.08558217	2.71468914
H	2.39951701	-1.10372373	2.12096417
H	0.04395590	1.04214105	3.09902895
H	-2.27886473	0.39120177	2.53465909
H	-1.08444722	-0.35742206	-1.50975342

H	1.24588053	0.24810961	-0.94141803
H	1.22616199	3.35777320	1.05953468
H	0.74150227	5.41807387	-0.16904453
H	1.92506232	5.93811985	-2.29157405
H	3.62388705	4.33960816	-3.15277176
H	4.12975027	2.26690597	-1.91762410
H	4.23299112	-2.62450586	2.18732494
H	5.57103234	-4.62970894	1.68434171
H	6.74669353	-4.83179949	-0.48958901
H	6.57276572	-3.00403219	-2.15708642
H	5.22806211	-0.99006881	-1.65425245
C	-4.94498524	-1.58773073	-0.58724010
C	-5.58186534	-2.70220723	-1.13662870
C	-4.81753924	-3.79951028	-1.50304184
C	-5.41671209	-0.31265807	-0.08819262
C	-6.67794605	0.27945147	-0.00034031
C	-6.78360650	1.55993041	0.52105475
C	-5.64128094	2.25428522	0.94715245
C	-4.37705899	1.68813077	0.87245348
H	-7.56002070	-0.25402924	-0.33839262
H	-7.75541067	2.03328439	0.59821265
H	-5.74632437	3.25795143	1.34337296
H	-3.49872176	2.23574673	1.19325763
C	-3.42663805	-3.79532682	-1.31789674
C	-2.76947957	-2.70057522	-0.77575401
H	-6.65822335	-2.70875295	-1.27148649
H	-5.29571888	-4.67154550	-1.93321525
H	-2.84943211	-4.66772960	-1.60301307
H	-1.69600987	-2.70867187	-0.62903139

Cz-TPP T₁ state

C	0.90631500	0.64002800	1.14413500
N	3.12231600	1.37783200	0.34922900
C	2.34481700	0.93042800	1.51924900
C	3.12630200	-0.33186200	1.92244600
C	3.80128200	-0.68847000	0.63609500
N	3.91534200	0.45609700	-0.20888000
C	4.26407700	-1.93198000	0.22212200
C	2.97196600	2.63182800	-0.23818200
C	-0.12596200	0.97182400	2.01854700
C	-1.44427900	0.66222200	1.70718000
C	-1.73997200	0.03342400	0.49981900
C	-0.71365100	-0.29081300	-0.38688300
C	0.60262500	0.00465100	-0.06077000

N	-3.08342900	-0.26785500	0.16816100
C	2.05874200	3.56092300	0.28319300
C	1.93664400	4.81000200	-0.30854900
C	2.70635000	5.15057300	-1.41764000
C	3.60741100	4.22215400	-1.93586400
C	3.74536200	2.96891500	-1.35974200
C	4.18889300	-3.08538700	1.06544400
C	4.65319800	-4.30681600	0.63178400
C	5.21474900	-4.45087900	-0.64686400
C	5.30553900	-3.33445100	-1.48553900
C	4.85082100	-2.09863100	-1.07302900
C	-3.56675000	-1.51806200	-0.20782000
C	-4.13929700	0.63928200	0.15285900
H	2.38664200	1.70025300	2.29148900
H	3.85372100	-0.08516100	2.70468500
H	2.46745900	-1.11216500	2.30335500
H	0.09861500	1.46679700	2.95820300
H	-2.24549500	0.90031200	2.39755600
H	-0.95350000	-0.75884000	-1.33489100
H	1.39484900	-0.23746200	-0.76308200
H	1.43680500	3.31345100	1.13381500
H	1.22721100	5.52042000	0.10001800
H	2.60178700	6.12699700	-1.87551600
H	4.20972000	4.47623400	-2.80070800
H	4.44235100	2.24325700	-1.75484800
H	3.76809700	-2.99279700	2.06079500
H	4.58710000	-5.16722800	1.28904700
H	5.57876100	-5.41603900	-0.97818700
H	5.74271500	-3.43956600	-2.47295900
H	4.92813300	-1.23615900	-1.72299700
C	-4.95039600	-1.41634400	-0.46449600
C	-5.66933800	-2.55097300	-0.84499900
C	-5.00258900	-3.76113000	-0.95861800
C	-5.31702300	-0.03447200	-0.23405900
C	-6.51684000	0.67131600	-0.33806700
C	-6.52215700	2.03020500	-0.06298100
C	-5.33922600	2.68819400	0.30602800
C	-4.13446600	2.00939300	0.41801500
H	-7.42838400	0.16296200	-0.63382500
H	-7.44525500	2.59290200	-0.13719400
H	-5.36342200	3.75330700	0.50649600
H	-3.22415100	2.52887700	0.69256700
C	-3.62864500	-3.84759800	-0.68789800
C	-2.89157900	-2.73525000	-0.30781100

H	-6.73361200	-2.48515300	-1.04445700
H	-5.54573800	-4.65111900	-1.25396800
H	-3.12886300	-4.80568500	-0.77550300
H	-1.83269000	-2.81438000	-0.09210400