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Supplementary Information

Nitrogen Analogues of Chichibabin's and Müller's Hydrocarbons with Small Singlet-Triplet Energy gaps

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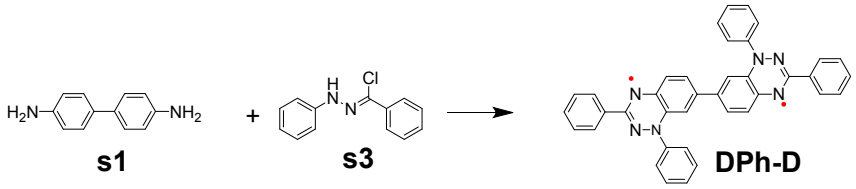
1. Methods and Materials

All reagents were purchased from Sigma-Aldrich, Acros and Adamas and used as received. Flash column chromatography was performed with Haiyang silica gel (200-300 mesh), and Greagent neutral Aluminium Oxide (200-300 mesh). Solvent tetrahydrofuran (THF) was freshly distilled from Na under N_2. All reaction mixtures and column eluents were monitored by TLC using commercial Huanghai glass plates (HSGF 254, 2.5 x 8 cm). The plates were visualized under UV radiation at 254 and 365 nm. UV/Vis/NIR absorption spectra were recorded on a Shimadzu UV-2600 UV-VIS spectrophotometer. High resolution mass spectra (HRMS) were measured on a Waters-Q-TOF-Premier (ESI). MALDI-TOF mass spectra (MS) were recorded on a SHIMADZU iD plus Performance using anthracene-1, 8, 9-triol as matrix. ESR measurements were carried out on a Bruker EMX plus X-band spectrometer with 9.8 GHz microwave frequency. SQUID measurements were carried out on a Quantum Design (MPMS-SQUID VSM-094). Thermogravimetric analysis (TGA) measurements were performed on NETZSCH TG 209F1 Iris thermal gravimetric analyzer. Fourier transform infrared (FT-IR) spectra were measured on a Thermo Fisher Scientific Nicolet 6700 spectrometer. Elemental analysis measurements were performed on a Leeman Labs Euro EA 3000 elemental analyzer. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation.

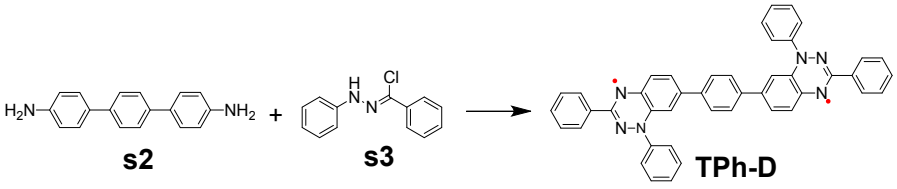
2. Preparation of diradicaloids DPh-D and TPh-D

Synthesis of DPh-D



To an anhydrous THF solution (20 mL) of 4,4′-diaminobiphenyl **s1** (0.4 g, 2.0 mmol) and (Z)-1-[Chloro(phenyl)-methylene]-2-phenyl-hydrazine **s3**[1] (1.0 g, 4.3 mmol) was added TEA (1 mL) at room temperature. Then the mixture was heated to reflux for 24 h, monitored by TLC. The resulting mixture was cooled to room temperature and the precipitate was removed by suction filtration, followed by evaporation of THF under a reduced pressure. The residue was dissolved in dry DCM (20 ml) and treated with 1,8-diazabicyclo[5.4.0]undec-7-ene DBU (0.5 ml) and 10 wt% Pd/C powder (50 mg). Then this solution was stirred exposed to air, after 24 h the solution was filtered and evaporated to yield a crude black solid. This solid was purified by triethylamine pretreated column chromatography (SiO_2, EtOAc: Hexane = 1: 8 to 1: 5) and recrystallized from CH_2Cl_2/Hexane to give the diradical **DPh-D** as a black solid (63.0 mg, 6%). HRMS (ESI^+): calcd. for $C_{38}H_{26}N_6^{2\bullet}$ 566.2219, found $[M+H]^+$ 567.2264. Element analysis (%) calcd. C 80.54 H 4.62, N 14.83; found C 80.45, H 4.66, N 14.88. IR (KBr, cm^{-1}) 3060, 1592, 1537, 1488, 1450, 1398, 1316, 1275, 1170, 1144, 1073, 1052, 1028.

Synthesis of TPh-D



To an anhydrous THF solution (20 mL) of 4,4″-diamino-p-terphenyl **s2** (0.4 g, 1.5 mmol) and **s3**[1] (830.0 mg, 3.6 mmol) was added TEA (1 mL) at room temperature. Then the mixture was heated to reflux for 24 h, monitored by TLC. The resulting mixture was cooled to room temperature and the precipitate was removed by suction filtration, followed by evaporation of THF under a reduced pressure. The residue was dissolved in dry DCM (20 ml) and treated with DBU (0.5 ml) and 10 wt% Pd/C powder (50 mg). Then this solution was stirred exposed to air, after 24 h the solution was filtered and evaporated to yield a crude black solid. This solid was purified by triethylamine pretreated column chromatography (SiO_2, EtOAc: Hexane = 1: 5) and recrystallized from CH_2Cl_2/Hexane to give the diradical **TPh-D** as a dark solid (130.0 mg, 14%). HRMS (ESI^+): calcd. for $C_{44}H_{30}N_6^{2\bullet}$ 642.6532, found $[M+H]^+$ 643.2573. Element analysis (%) calcd. C 82.22 H 4.70, N 13.08; found C 82.30, H 4.65, N 13.05. IR (KBr, cm^{-1}) 3024, 1593, 1527, 1485, 1448, 1391, 1351, 1314, 1232, 1200, 1166, 1117, 1063, 1023, 1000.

3. Mass spectra

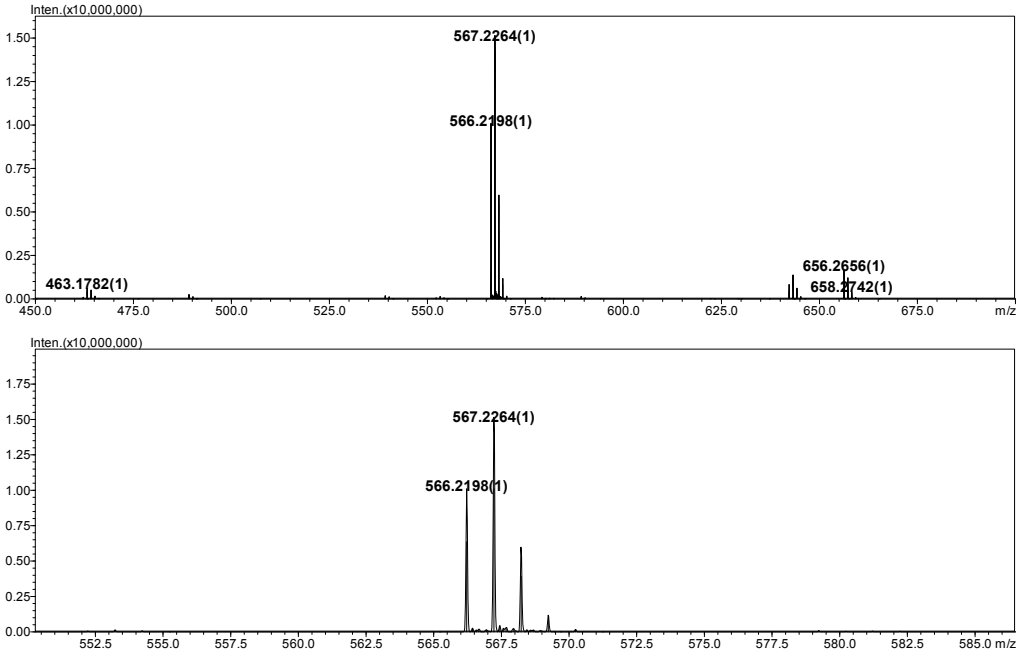


Figure S1. Mass spectra of **DPh-D** (ESI+).

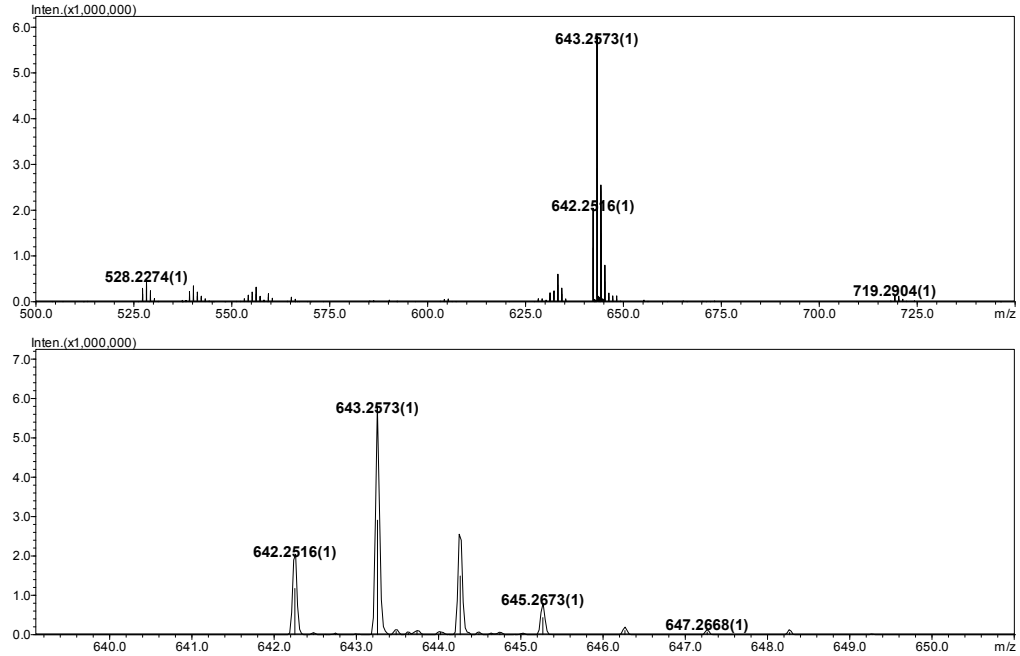


Figure S2. Mass spectra of **TPh-D** (ESI+)..

4. The calculation of energy gaps

Optical energy gaps

UV/vis/NIR absorption spectra (**Figure S3**) reveal that the absorption onsets are 1016 and 739 nm for **DPh-D** and **TPh-D**, respectively. The corresponding optical energy gaps Eg^{Opt} are 1.22 and 1.68 eV for **DPh-D** and **TPh-D**, respectively.

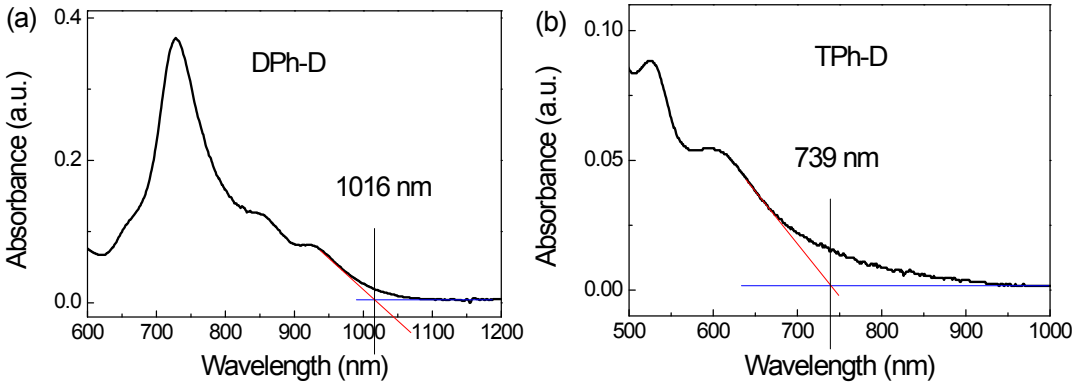


Figure S3. The partial UV/vis/NIR absorption spectra of **DPh-D** (a), and **TPh-D** (b) in DCM. The cross indicates the onset of each compound.

Electrochemical energy gaps

Cyclic voltammograms were measured in dry DCM with 0.1 M Bu_4NPF_6 as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 100 mV/s. The HOMO and LUMO energy levels of both compounds were estimated from the half-wave potential $E_{1/2}$ in **Figure 3** using ferrocene (**Figure S4**) as reference. The equations used to calculate the energy level are: HOMO = - (E^{ox}_{sample} - $E^{ox}_{Fc/Fc+}$ + 4.8), LUMO = - (E^{red}_{sample} – $E^{red}_{Fc/Fc+}$ + 4.8). The yield values for HOMO and LUMO energy levels are summarized in **Table 1**.

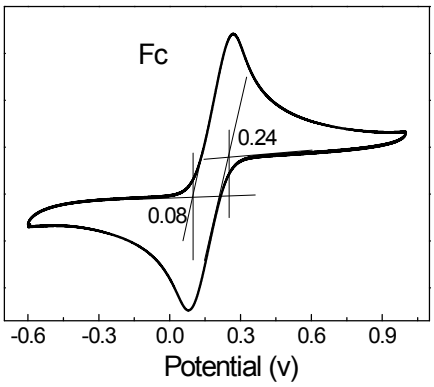


Figure S4. Cyclic voltammograms of ferrocene in dry DCM with 0.1 M Bu_4NPF_6 as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 100 mV/s.

5. Open circuit potential

The open circuit potential (**Figure S5**) was measured in dry DCM with 0.1 M Bu_4NPF_6 as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, a sample interval of 2 sec, and a scan time of 100 sec. The open circuit potential values of **DPh-D** and **TPh-D** are 0.12 and 0.10 V, respectively.

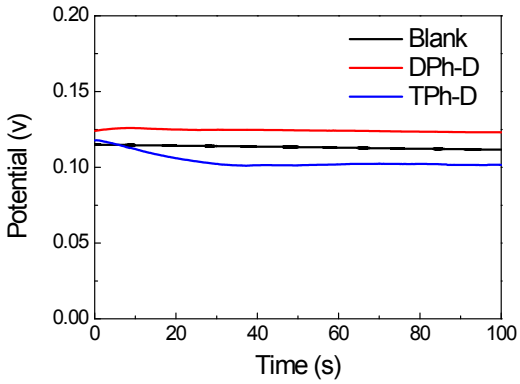


Figure S5. The change of open circuit potential of **DPh-D and TPh-D** in dry DCM as a function of scan time with a sample interval of 2 sec, and a scan time of 100 sec.

6. X-ray crystallography

Black single crystals of **DPh-D** were grown by allowing slow evaporation of a nearly saturated solution of **DPh-D** in DCM at room temperature. Unfortunately, single crystals of **TPh-D** could not be obtained by accessing many methods, only amorphous powders were formed.

DPh-D has centrosymmetric and planar core backbone (**Figure S5**), and the phenyl at the N3 position is twisted relative to the core plane with a dihedral angle of c.a. 58.5°. The torsion angle between the phenyl at C7(a) position and the triazinyl ring is 19.5°.

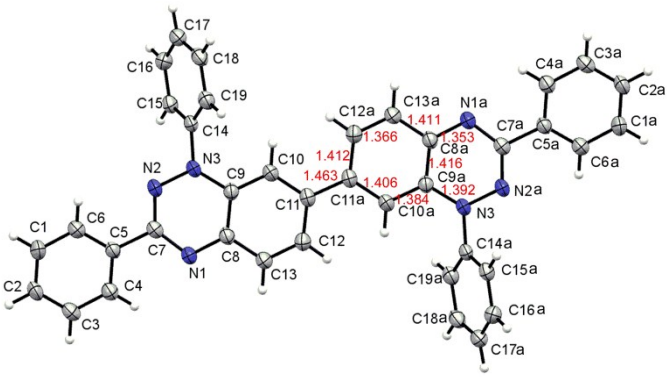


Figure S6. Single-crystal X-ray structure of **DPh-D** with selected bond lengths (Å) with thermal ellipsoids shown at the 50% probability level.

Table S1. Sample and crystal data for **DPh-D**.

Identification code	**DPh-D**
Chemical formula	$C_{38}H_{26}N_6$
Formula weight	566.65 g/mol
Temperature	150 K
Wavelength	1.54184 Å
Crystal size	0.005 x 0.020 x 0.100 mm
Crystal system	triclinic

Space group	P -1
Unit cell dimensions	a = 6.0606(11) Å α = 90.724(17)°
	b = 8.5904(19) Å β = 93.870(16)°
	c = 13.007(3) Å γ = 96.893(18)°
Volume	670.6(2) $Å^3$
Z	1
Density (calculated)	1.408 g/cm^3
Absorption coefficient	0.667 mm^{-1}
F(000)	298

Table S2. Data collection and structure refinement for **DPh-D**.

Theta range for data collection	3.41 to 66.65°
Index ranges	-7<=h<=7, -9<=k<=10, -15<=l<=15
Reflections collected	7165
Independent reflections	2346 [R(int) = 0.0469]
Max. and min. transmission	1.0000 and 0.6000
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2346 / 0 / 200
Goodness-of-fit on F^2	1.073
Final R indices	1687 data; I>2σ(I) R1 = 0.0475, wR2 = 0.1351
	all data R1 = 0.0692, wR2 = 0.1509
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0644P)^2+0.3004P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0037(11)
Largest diff. peak and hole	0.254 and -0.189 $eÅ^{-3}$
R.M.S. deviation from mean	0.048 $eÅ^{-3}$

Table S3. Bond lengths (Å) for **DPh-D**.

N1-C8	1.353(3)	N1-C7	1.356(3)
C1-C2	1.380(4)	C1-C6	1.389(3)
C1-H1	0.94	N2-C7	1.317(3)
N2-N3	1.375(2)	C2-C3	1.378(4)

C2-H2	0.94	C3-C4	1.383(3)
C3-H3	0.94	N3-C9	1.392(3)
N3-C14	1.431(3)	C4-C5	1.388(3)
C4-H4	0.94	C5-C6	1.388(3)
C5-C7	1.483(3)	C6-H6	0.94
C8-C13	1.411(3)	C8-C9	1.416(3)
C10-C9	1.384(3)	C10-C11	1.406(3)
C10-H10	0.94	C11-C12	1.412(3)
C11-C11	1.463(4)	C12-C13	1.366(3)
C12-H12	0.94	C13-H13	0.94
C14-C19	1.380(3)	C14-C15	1.390(3)
C15-C16	1.377(3)	C15-H15	0.94
C16-C17	1.380(4)	C16-H16	0.94
C17-C18	1.390(4)	C17-H17	0.94
C18-C19	1.390(3)	C18-H18	0.94
C19-H19	0.94		

Table S4. Bond angles (°) for **DPh-D**.

C8-N1-C7	115.53(19)	C2-C1-C6	120.5(2)
C2-C1-H1	119.7	C6-C1-H1	119.7
C7-N2-N3	116.19(19)	C3-C2-C1	119.8(2)
C3-C2-H2	120.1	C1-C2-H2	120.1
C2-C3-C4	120.0(2)	C2-C3-H3	120.0
C4-C3-H3	120.0	N2-N3-C9	122.59(18)
N2-N3-C14	112.86(17)	C9-N3-C14	124.52(17)
C3-C4-C5	120.7(2)	C3-C4-H4	119.6
C5-C4-H4	119.6	C4-C5-C6	119.0(2)
C4-C5-C7	118.8(2)	C6-C5-C7	122.2(2)
C5-C6-C1	119.9(2)	C5-C6-H6	120.0
C1-C6-H6	120.0	N1-C8-C13	119.6(2)
N1-C8-C9	122.9(2)	C13-C8-C9	117.5(2)
N2-C7-N1	127.30(19)	N2-C7-C5	115.8(2)
N1-C7-C5	116.90(19)	C9-C10-C11	121.4(2)
C9-C10-H10	119.3	C11-C10-H10	119.3
C10-C11-C12	117.0(2)	C10-C11-C11	122.1(3)

C12-C11-C11	120.8(3)	C13-C12-C11	122.1(2)
C13-C12-H12	118.9	C11-C12-H12	118.9
C12-C13-C8	121.0(2)	C12-C13-H13	119.5
C8-C13-H13	119.5	C19-C14-C15	120.8(2)
C19-C14-N3	120.9(2)	C15-C14-N3	118.2(2)
C16-C15-C14	119.5(2)	C16-C15-H15	120.3
C14-C15-H15	120.3	C15-C16-C17	120.6(2)
C15-C16-H16	119.7	C17-C16-H16	119.7
C16-C17-C18	119.7(2)	C16-C17-H17	120.2
C18-C17-H17	120.2	C17-C18-C19	120.2(2)
C17-C18-H18	119.9	C19-C18-H18	119.9
C14-C19-C18	119.2(2)	C14-C19-H19	120.4
C18-C19-H19	120.4	C10-C9-N3	123.7(2)
C10-C9-C8	120.9(2)	N3-C9-C8	115.40(19)

Table S5. Torsion angles (°) for **DPh-D**.

C6-C1-C2-C3	0.0(4)	C1-C2-C3-C4	-0.6(4)
C7-N2-N3-C9	0.6(3)	C7-N2-N3-C14	-177.6(2)
C2-C3-C4-C5	1.4(4)	C3-C4-C5-C6	-1.4(4)
C3-C4-C5-C7	179.0(2)	C4-C5-C6-C1	0.7(4)
C7-C5-C6-C1	-179.7(2)	C2-C1-C6-C5	0.0(4)
C7-N1-C8-C13	-179.2(2)	C7-N1-C8-C9	0.4(3)
N3-N2-C7-N1	2.2(4)	N3-N2-C7-C5	-177.4(2)
C8-N1-C7-N2	-2.7(4)	C8-N1-C7-C5	176.9(2)
C4-C5-C7-N2	-160.9(2)	C6-C5-C7-N2	19.5(3)
C4-C5-C7-N1	19.5(3)	C6-C5-C7-N1	-160.1(2)
C9-C10-C11-C12	-1.8(3)	C9-C10-C11-C11	178.7(3)
C10-C11-C12-C13	0.8(4)	C11-C11-C12-C13	-179.6(3)
C11-C12-C13-C8	0.5(4)	N1-C8-C13-C12	178.8(2)
C9-C8-C13-C12	-0.8(4)	N2-N3-C14-C19	-120.5(2)
C9-N3-C14-C19	61.4(3)	N2-N3-C14-C15	55.6(3)
C9-N3-C14-C15	-122.6(2)	C19-C14-C15-C16	1.6(3)
N3-C14-C15-C16	-174.5(2)	C14-C15-C16-C17	0.5(3)
C15-C16-C17-C18	-2.3(4)	C16-C17-C18-C19	2.1(3)
C15-C14-C19-C18	-1.8(3)	N3-C14-C19-C18	174.1(2)

C17-C18-C19-C14	0.0(3)	C11-C10-C9-N3	179.7(2)
C11-C10-C9-C8	1.5(4)	N2-N3-C9-C10	179.3(2)
C14-N3-C9-C10	-2.7(4)	N2-N3-C9-C8	-2.4(3)
C14-N3-C9-C8	175.6(2)	N1-C8-C9-C10	-179.8(2)
C13-C8-C9-C10	-0.2(3)	N1-C8-C9-N3	1.9(3)
C13-C8-C9-N3	-178.5(2)		

7. Fourier transform infrared (IR) spectra

Before FT-IR measurements, the two diradicaloids were dried in vacuum at 50 °C for 48 hours, and the potassium bromide (KBr) was grinded to fine powders using an agate mortar then dried in oven at 150 °C for 4 hours. Then the mixture of each diradicaloid (~3 mg) and KBr (~150 mg) was grinded for 3-5 minutes under an infrared lamp. Finally, thin pellets were obtained by pressing the mixture under 10 MPa for 1 minute. The absence of typical N-H stretching vibration absorption above 3100 cm^{-1} indicates that all starting materials **s1** and **s2** are fully converted into the corresponding diradicals **DPh-D**, and **TPh-D**.

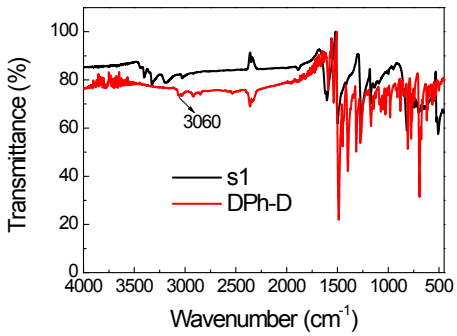


Figure S7. FT-IR spectra of compounds **s1** & **DPh-D**.

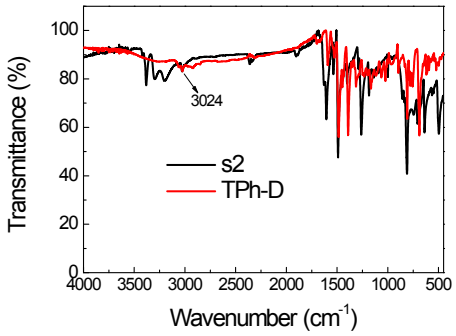


Figure S8. FT-IR spectra of compounds **s2** & **TPh-D**.

8. Magnetization measurements and data analysis

SQUID measurements

For SUQID measurements, first the two diradicaloids are dried in vacuum at 50 °C for 48 hours, then confirmed by Mass Spectra, FT-IR and combustion analyses. Magnetic susceptibility of powder samples of **DPh-D** (16.1 mg), and **TPh-D** (23.4 mg) was measured in a polycarbonate capsule fitted in a plastic straw as a function of temperature in heating (2 K→ 300 K) mode with 30 seconds of temperature stability at each temperature (1 K increment in a range 2–10 K, 3 K increment in a range 10–300 K,) at 1.0 T using a SQUID magnetometer (Quantum Design MPMS-SQUID VSM-094). The data was corrected for both sample diamagnetism (Pascal′s constants) and the diamagnetism of the sample holder (polycarbonate capsule) (**Figure S9**).

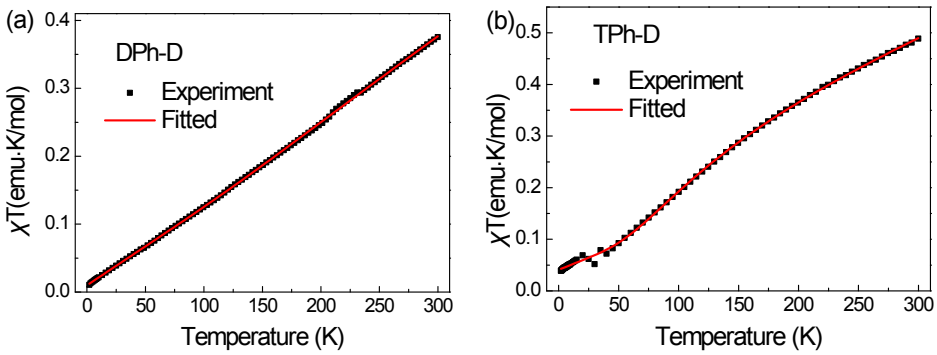


Figure S9. Temperature-dependent plots of χT for **DPh-D** (a) and **TPh-D** (b) measured at 1.0 T in the stable mode from 2 to 300 K. The solid lines are the fitting curves according to Bleaney−Bowers equation (inset); g-factor was taken to be 2.

SQUID Data analysis

The SQUID data in **Figure S9** were fitted with a modified Bleaney-Bowers equation.[2] The yield singlet-triplet energy gap ($\Delta E_{S\text{-}T}$) of -1.15 and -0.50 kcal/mol for **DPh-D** and **TPh-D**, respectively, with the Adj. R-Square >0.99. The tendency of $\Delta E_{S\text{-}T}$ values for powder samples is in agreement with that of solid solution samples (**Table 1**), and the smaller values are due to the intermolecular interactions.

ESR simulation

Simulations of ESR spectra were performed with the *Easyspin* program in Matlab.[3]

9. Computational details

All calculations were performed with the Gaussian 16 program suite.[4] Full geometry optimizations were carried out at the (U)B3LYP/6–31G(d) level,[5] and the obtained stationary points were characterized by frequency calculations. The diradical character *y* was calculated by a symmetry-broken UB3LYP/6-31G(d) method, basing on the LUMO occupation number (nLUMO) in natural orbital analysis for the optimized singlet geometry. The y is formally expressed as $y = 1 - (2T/(1 + T^2))$, where T is represented by calculating the occupation numbers of natural orbitals as: T = (nHOMO – nLUMO)/2. A molecule with y = 0 implies a closed-shell structure, whereas a molecule with y = 1 indicates a pure diradical structure. Any intermediate value of y refers to diradicaloid (i.e. diradical like) structures.[6] The HOMO and LUMO orbitals of **DPh-D** and **TPh-D** OS state were delocalized mainly at the

backbone of benzotriazinyl moiety. The spin densities were illustrated using Multiwfn and VMD.[7]

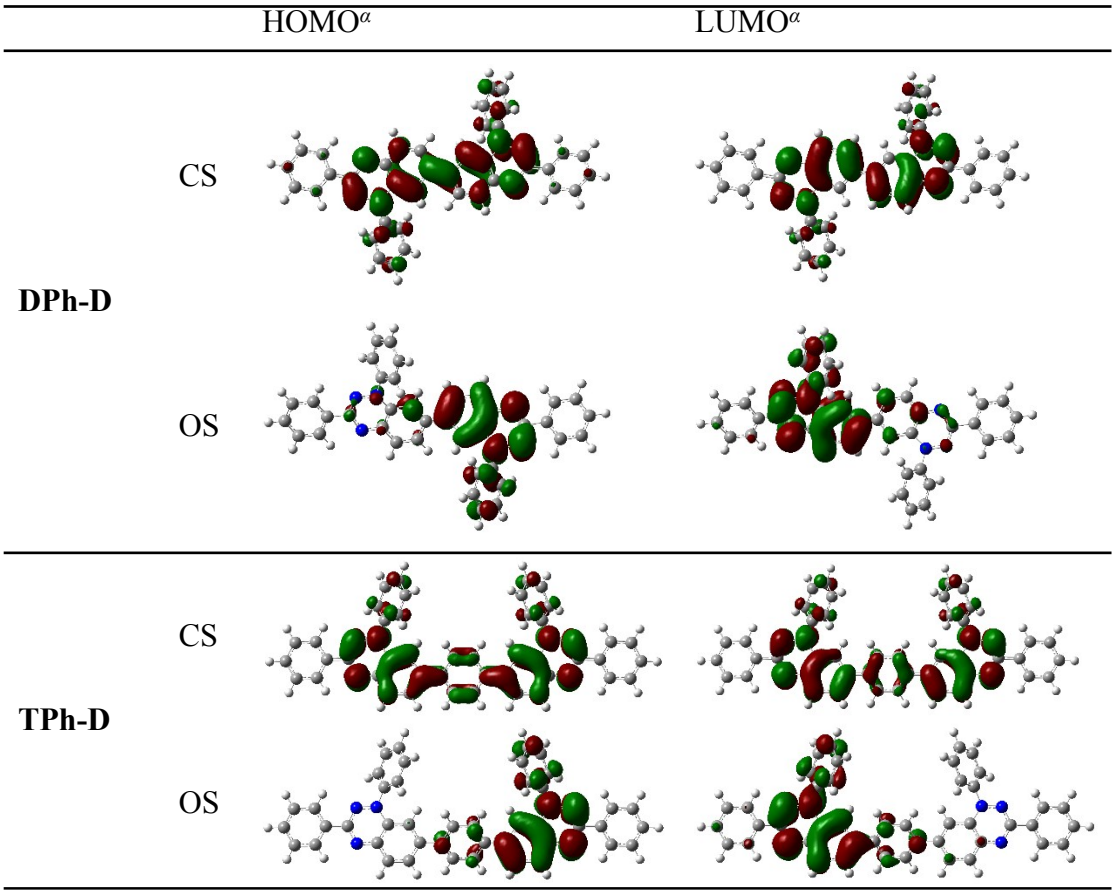


Figure S10. Frontier orbitals of **DPh-D** and **TPh-D** calculated at the UB3LYP/6-31G(d) level ($^{\alpha}$HOMO(α) and LUMO(α) for the OS states).

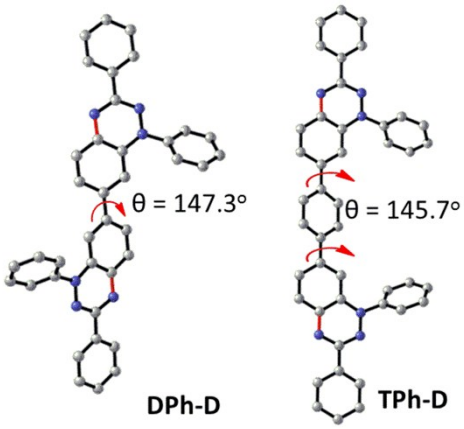


Figure S11. The optimized structures of **DPh-D** and **TPh-D** in the open-shell singlet diradical ground state calculated at the UB3LYP/6-31G(d) level.

Table S6. Selected calculated relative energy (kcal/mol), bond lengths (Å), and dihedral (°) of **DPh-D** and **TPh-D**.

Compounds	States	ΔE[a]	avg. d_1&d_2[b]	θ
DPh-D	CS	8.029	1.327	162.0
	OS	0	1.361	147.3
	T	0.799	1.366	145.1
TPh-D	CS	14.344	1.339	160.2
	OS	0	1.364	145.7
	T	0.154	1.365	144.9

[a] Energy relative to the OS state. CS=closed-shell singlet, OS=open-shell singlet. [b] The red colored bonds.

10.Stability test

Chemical stability

The solid forms of both diradicaloids are stable for more than one year under ambient conditions without noticeable degradation. The DCM solutions of these compounds are stable for more than two months without significate decomposition (**Figure S12**).

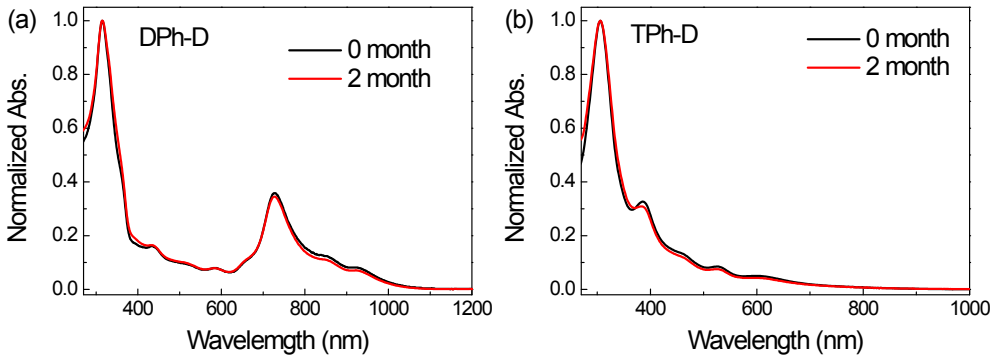


Figure S12. UV/vis/NIR absorption spectra of **DPh-D** (a), and **TPh-D** (b) in DCM for different time.

Thermal stability

TGA diagram (**Figure S13**) indicates that **DPh-D** is stable up to ~ 290 °C, while **TPh-D** is stable up to ~ 160 °C. To verify whether these diradicaloids remain intact at high temperature, we annealed the powder samples of them at different temperatures for 15 minutes under N_2 using the TGA apparatus. The UV-Vis-NIR measured in DCM after each step of annealing and MS spectra (**Figure S14**) reveal that **DPh-D** is stable up to 250 °C without any decomposition, it begins decompose at 300 °C. While the less stable **TPh-D** (**Figure S15**) is stable up to 150 °C without obvious decomposition, it begins decompose at 175 °C.

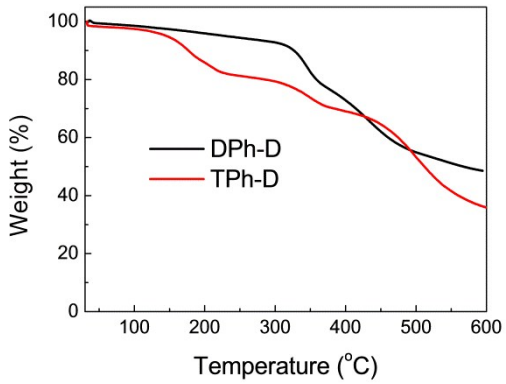


Figure S13. TGA of **DPh-D** and **TPh-D** under N_2; heating rate = 10 °C/min.

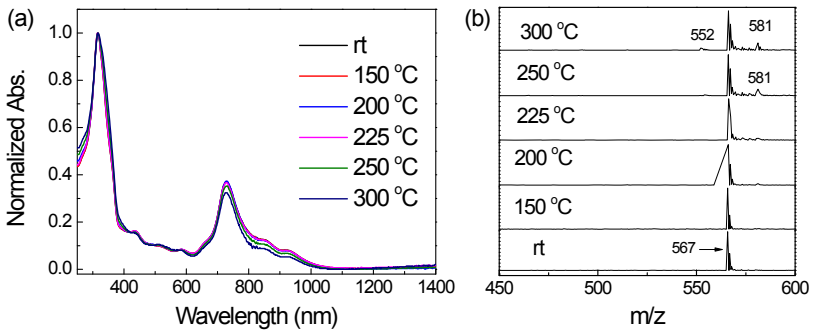


Figure S14. Room temperature UV-Vis-NIR absorption spectra (a) in DCM and MALDI-TOF mass spectra (b) of **DPh-D** after annealing for different temperatures under N2 for 15 minutes (using TGA apparatus).

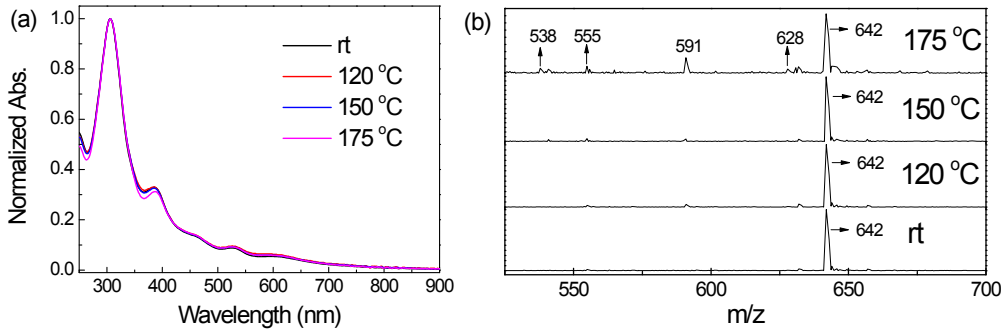


Figure S15. Room temperature UV-Vis-NIR absorption spectra (a) in DCM and MALDI-TOF mass spectra (b) of **TPh-D** after annealing for different temperatures under N2 for 15 minutes (using TGA apparatus).

Photo stability

The Photo stability was studied in DCM upon irradiation with a white light (400 W), and the distance between sample and lamp is 20 cm. The yield half-life ($t_{1/2}$) was 503.8 h (728 nm) for **DPh-D**, and 20.4 h (306 nm) for **TPh-D**.

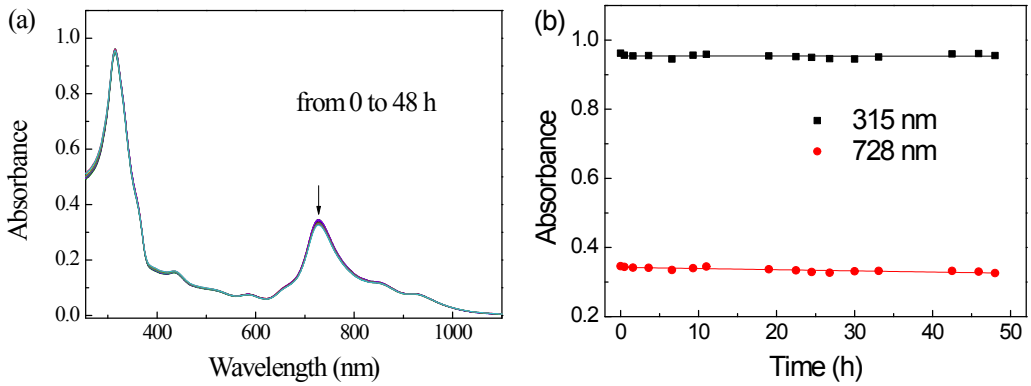


Figure S16. UV-Vis-NIR absorption spectra of **DPh-D** (a) in DCM upon irradiation with white light (400 W). The changes of the optical density at 315 and 728 nm for **DPh-D** (b) as a function of irradiation time.

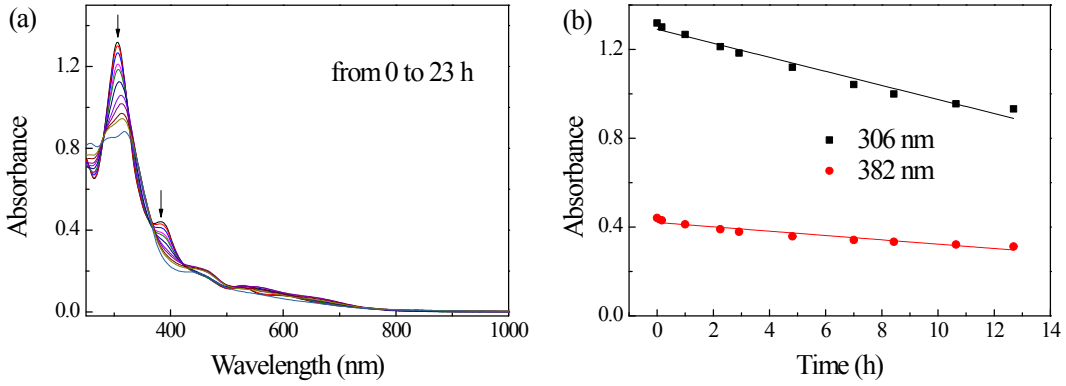


Figure S17. UV-Vis-NIR absorption spectra of **TPh-D** (a) in DCM upon irradiation with white light (400 W). The changes of the optical density at 306 and 382 nm for **TPh-D** (b) as a function of irradiation time.

11.Supporting References

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12. Coordinates for calculated geometries:

DPh-D CS

C	-5.63717800	-0.70252900	-0.29919700
N	-5.48419600	0.56771600	0.00164400
N	-4.21576000	1.01921200	0.22632200
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C	-1.78252300	0.66435000	0.02681200
C	-0.68337900	-0.22546700	-0.14182700
C	-0.99812400	-1.60987200	-0.33442200
C	-2.28626700	-2.06434300	-0.39633800
C	-4.15166300	2.39065600	0.61727200
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DPh-D OS

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H	2.66776800	-1.78961000	2.31860200
H	7.89516300	-0.76770900	0.11952900
H	10.24573500	-0.04324500	-0.20665200
H	10.73703200	2.24333100	-1.05460100

H	8.86257800	3.79498900	-1.57228100
H	6.51005900	3.05230800	-1.24167100

DPh-D T

C	-5.63611800	-0.66768600	-0.37013500
N	-5.44825600	0.58761800	0.05435800
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C	-3.39615600	-1.13768100	-0.54289600
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C	-1.74357200	0.62956400	-0.13968500
C	-0.70156600	-0.23728300	-0.49842200
C	-1.02233900	-1.56487700	-0.86106400
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C	2.33570900	1.99919600	-0.88811400

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C	3.07186400	-0.18802200	-0.13232000
C	1.74360200	-0.62948800	-0.13966400
N	4.68775100	1.57454000	-0.63449200
C	5.63616600	0.66767500	-0.37012300
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N	4.15682500	-0.98703700	0.24012700
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C	7.05541800	1.07831700	-0.54327900
C	4.79755300	-3.34027600	0.22984100
C	4.70652900	-4.62298600	0.76568100
C	3.85635200	-4.88067600	1.84384700
C	3.10288800	-3.84219100	2.39393700
C	3.19064000	-2.55277700	1.86977700
C	8.10925200	0.20780000	-0.22312100
C	9.43151700	0.61049300	-0.39598100
C	9.72081900	1.88533000	-0.88884100
C	8.67689400	2.75646400	-1.20750400
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H	-0.22999600	-2.24189800	-1.16493000
H	-2.59275800	-3.00620600	-1.20034300
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H	1.51375900	-1.64510600	0.15590200
H	5.45878200	-3.12402200	-0.60161000
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H	7.88016300	-0.77881200	0.16360600
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H	8.89422700	3.74990400	-1.59113600
H	6.53337700	3.02439200	-1.27991300

TPh-D CS

C	7.72608500	-0.59057000	-0.10538200
N	7.15965500	0.60172100	-0.14858300
N	5.81135700	0.66225700	0.05967500
C	5.02072200	-0.48538200	0.14889800
C	5.75903600	-1.72123600	0.22039800
N	7.09360900	-1.77119400	0.12516800
C	3.63127100	-0.48891800	0.12871300
C	2.89676400	-1.69099800	0.25193400
C	3.63510300	-2.90127500	0.38530400
C	5.00891400	-2.91932400	0.37136000
C	9.19584400	-0.63190600	-0.31707600
C	5.29237200	1.99031200	0.10474500

C	1.44090000	-1.69752200	0.25801200
C	0.69037100	-2.85926500	-0.05251300
C	-0.69031600	-2.85927200	-0.05256100
C	-1.44089000	-1.69754100	0.25791400
C	-0.69013600	-0.53604700	0.57008900
C	0.69011400	-0.53603700	0.57013300
C	-2.89675600	-1.69104700	0.25173400
C	-3.63509400	-2.90135000	0.38486800
C	-5.00890400	-2.91938700	0.37089700
C	-5.75902700	-1.72127100	0.22017100
C	-5.02072000	-0.48541000	0.14879400
C	-3.63127300	-0.48895000	0.12866600
N	-7.09360500	-1.77123300	0.12498800
C	-7.72609000	-0.59058900	-0.10544000
N	-7.15965600	0.60170200	-0.14858700
N	-5.81136800	0.66223500	0.05967300
C	-5.29237100	1.99028500	0.10470300
C	-9.19586200	-0.63189200	-0.31702500
C	9.93747700	0.54589400	-0.50473000
C	11.31393400	0.48619600	-0.70468200
C	11.97127500	-0.74731500	-0.72007000
C	11.24016400	-1.92138700	-0.53246800
C	9.86161800	-1.86657200	-0.33178300
C	4.38925200	2.37020100	1.10665900
C	3.92165200	3.68233800	1.15288700
C	4.35358800	4.62141500	0.21375300
C	5.26693400	4.24074200	-0.77219300
C	5.73960000	2.93181600	-0.83064200
C	-4.38923600	2.37018600	1.10659800
C	-3.92160800	3.68231500	1.15278800

C	-4.35353500	4.62137800	0.21363700
C	-5.26690400	4.24069700	-0.77228400
C	-5.73959600	2.93177900	-0.83069600
C	-9.93753100	0.54594600	-0.50429300
C	-11.31400400	0.48628000	-0.70414700
C	-11.97132700	-0.74723700	-0.71981400
C	-11.24018000	-1.92134900	-0.53259100
C	-9.86161900	-1.86656600	-0.33200700
H	3.10506300	0.44385100	-0.02343400
H	3.10282100	-3.83576300	0.52840700
H	5.56757100	-3.84485800	0.46339400
H	1.20424000	-3.76767500	-0.35003000
H	-1.20414300	-3.76769300	-0.35011200
H	-1.20649500	0.37197800	0.86514300
H	1.20645200	0.37199200	0.86521300
H	-3.10283100	-3.83587400	0.52779300
H	-5.56758200	-3.84492700	0.46274800
H	-3.10504600	0.44382600	-0.02335900
H	9.42478000	1.50124600	-0.48737100
H	11.87694000	1.40494700	-0.84710000
H	13.04605700	-0.79122400	-0.87593500
H	11.74387800	-2.88445400	-0.54231600
H	9.28400500	-2.77178800	-0.18392700
H	4.07675300	1.64948600	1.85490200
H	3.22878300	3.97346200	1.93755000
H	3.98706900	5.64307700	0.25442300
H	5.61244400	4.96549300	-1.50413900
H	6.45430900	2.62654400	-1.58617500
H	-4.07675800	1.64949500	1.85487400
H	-3.22872200	3.97343900	1.93743600

H	-3.98699200	5.64303300	0.25427800
H	-5.61242000	4.96543300	-1.50424300
H	-6.45432200	2.62650900	-1.58621400
H	-9.42484900	1.50130200	-0.48671500
H	-11.87703500	1.40506000	-0.84626800
H	-13.04612100	-0.79112100	-0.87559700
H	-11.74387900	-2.88442100	-0.54265600
H	-9.28397900	-2.77181200	-0.18444600

TPh-D OS

C	7.72202300	-0.60065300	-0.10382000
N	7.14820300	0.60559400	-0.15360500
N	5.80014400	0.65440200	0.05288700
C	5.02184800	-0.50250300	0.15452500
C	5.74841100	-1.72781400	0.21604800
N	7.10880500	-1.77114700	0.12148400
C	3.62276700	-0.50465900	0.15020300
C	2.90662800	-1.70461300	0.26800500
C	3.63094200	-2.91330100	0.38203500
C	5.01318000	-2.92387600	0.35034800
C	9.19530400	-0.61924300	-0.30849000
C	5.26613500	1.97933300	0.09264600
C	1.42707200	-1.70256600	0.27071900
C	0.69487700	-2.76520800	-0.28955400
C	-0.69487200	-2.76520900	-0.28954600
C	-1.42706300	-1.70256900	0.27073700
C	-0.69489400	-0.63996800	0.83073000
C	0.69490800	-0.63996600	0.83072100
C	-2.90661800	-1.70461900	0.26803800

C	-3.63093200	-2.91331000	0.38205400
C	-5.01316900	-2.92388900	0.35036300
C	-5.74840300	-1.72782500	0.21607700
C	-5.02184400	-0.50251100	0.15460100
C	-3.62276300	-0.50466600	0.15026500
N	-7.10879300	-1.77116300	0.12147600
C	-7.72200200	-0.60067100	-0.10386700
N	-7.14818700	0.60558000	-0.15359100
N	-5.80014400	0.65439900	0.05300600
C	-5.26616600	1.97933100	0.09294200
C	-9.19527000	-0.61926800	-0.30862700
C	9.92083200	0.56973000	-0.48418300
C	11.29971800	0.53043400	-0.67754100
C	11.97364500	-0.69325200	-0.69724500
C	11.25782100	-1.87924900	-0.52125300
C	9.87819100	-1.84458500	-0.32818900
C	4.40366700	2.36767700	1.12467100
C	3.91764400	3.67416700	1.16176600
C	4.29603500	4.59648800	0.18435800
C	5.17153100	4.20691500	-0.83203800
C	5.65938400	2.90291800	-0.88218200
C	-4.40365300	2.36754400	1.12498100
C	-3.91766600	3.67404200	1.16225400
C	-4.29613300	4.59650600	0.18501200
C	-5.17167400	4.20706500	-0.83139600
C	-5.65949400	2.90306300	-0.88171800
C	-9.92080600	0.56970600	-0.48427600
C	-11.29968000	0.53040300	-0.67772400
C	-11.97358600	-0.69329200	-0.69755900
C	-11.25775500	-1.87929100	-0.52160900

C	-9.87813700	-1.84461900	-0.32845500
H	3.08575100	0.42608300	0.01660200
H	3.09250700	-3.84675800	0.51350000
H	5.57541800	-3.84938500	0.42179400
H	1.22221200	-3.58542400	-0.76789000
H	-1.22221200	-3.58542600	-0.76787700
H	-1.22268900	0.18107900	1.30749400
H	1.22270800	0.18108100	1.30747800
H	-3.09249500	-3.84676800	0.51350700
H	-5.57540400	-3.84940100	0.42178600
H	-3.08575100	0.42608100	0.01667800
H	9.39461400	1.51743400	-0.46310000
H	11.85067700	1.45779500	-0.81101500
H	13.04976400	-0.72149200	-0.84768700
H	11.77517900	-2.83501100	-0.53492500
H	9.31118500	-2.75817000	-0.19007900
H	4.13588600	1.65847500	1.90103800
H	3.25391400	3.97380900	1.96803600
H	3.91744000	5.61402900	0.21865400
H	5.47517200	4.92024400	-1.59311700
H	6.34585400	2.58916400	-1.66033900
H	-4.13581300	1.65823600	1.90123100
H	-3.25390400	3.97357400	1.96853800
H	-3.91756400	5.61405200	0.21944700
H	-5.47537800	4.92050200	-1.59234900
H	-6.34599600	2.58941400	-1.65988800
H	-9.39460400	1.51741700	-0.46308900
H	-11.85064500	1.45776500	-0.81116200
H	-13.04969500	-0.72153800	-0.84807100
H	-11.77509600	-2.83506000	-0.53538300

H	-9.31112600	-2.75820500	-0.19037500

TPh-D T

C	7.72137800	-0.60119100	-0.10537300
N	7.14719300	0.60568800	-0.15475600
N	5.79934200	0.65393600	0.05281500
C	5.02174300	-0.50318000	0.15591800
C	5.74792600	-1.72824800	0.21667800
N	7.10923600	-1.77123800	0.12041800
C	3.62221700	-0.50525900	0.15373500
C	2.90696400	-1.70510600	0.27258400
C	3.63076200	-2.91371400	0.38591500
C	5.01334500	-2.92406500	0.35188900
C	9.19453300	-0.61876100	-0.31134500
C	5.26483900	1.97873000	0.09247100
C	1.42641900	-1.70256200	0.27536400
C	0.69504500	-2.75815100	-0.29812400
C	-0.69509300	-2.75815200	-0.29808400
C	-1.42642100	-1.70256800	0.27545100
C	-0.69509900	-0.64698300	0.84849100
C	0.69512200	-0.64697500	0.84843900
C	-2.90698600	-1.70510500	0.27278000
C	-3.63078000	-2.91370700	0.38624000
C	-5.01336000	-2.92406000	0.35227100
C	-5.74794200	-1.72824300	0.21699400
C	-5.02176200	-0.50318500	0.15619000
C	-3.62223200	-0.50527200	0.15388400
N	-7.10924700	-1.77123200	0.12065700
C	-7.72131700	-0.60122500	-0.10556200

N	-7.14712800	0.60565000	-0.15494100
N	-5.79934600	0.65394200	0.05311200
C	-5.26493100	1.97872500	0.09355100
C	-9.19442600	-0.61882700	-0.31190800
C	9.91926300	0.57073400	-0.48667700
C	11.29802700	0.53232100	-0.68129700
C	11.97254200	-0.69098400	-0.70262000
C	11.25748800	-1.87753200	-0.52698700
C	9.87804000	-1.84373800	-0.33267900
C	4.40412200	2.36760300	1.12573300
C	3.91763200	3.67394000	1.16254200
C	4.29392600	4.59552300	0.18364600
C	5.16777600	4.20542500	-0.83397900
C	5.65607700	2.90159300	-0.88383600
C	-4.40385200	2.36689400	1.12677900
C	-3.91744400	3.67324200	1.16438500
C	-4.29415200	4.59553400	0.18632400
C	-5.16834600	4.20612300	-0.83127700
C	-5.65657900	2.90230400	-0.88193400
C	-9.91911300	0.57064400	-0.48756800
C	-11.29782400	0.53220400	-0.68255200
C	-11.97233100	-0.69110600	-0.70389600
C	-11.25732100	-1.87762900	-0.52792400
C	-9.87792200	-1.84380800	-0.33326400
H	3.08455800	0.42531600	0.02128800
H	3.09208900	-3.84702100	0.51766400
H	5.57572200	-3.84958500	0.42224600
H	1.22304700	-3.57254100	-0.78566800
H	-1.22311900	-3.57253400	-0.78562100
H	-1.22341600	0.16828900	1.33457000

H	1.22346800	0.16831600	1.33445400
H	-3.09210000	-3.84700500	0.51804100
H	-5.57574500	-3.84957000	0.42269000
H	-3.08459100	0.42530400	0.02132700
H	9.39256100	1.51812900	-0.46432000
H	11.84839100	1.46007600	-0.81447100
H	13.04854200	-0.71855400	-0.85404200
H	11.77534500	-2.83300300	-0.54193000
H	9.31157000	-2.75770100	-0.19482800
H	4.13813600	1.65898800	1.90325000
H	3.25522800	3.97404300	1.96972700
H	3.91501300	5.61295300	0.21774000
H	5.46978400	4.91821700	-1.59620600
H	6.34132100	2.58740300	-1.66289700
H	-4.13752100	1.65774500	1.90368900
H	-3.25477000	3.97277300	1.97156100
H	-3.91530100	5.61296500	0.22103000
H	-5.47067300	4.91946300	-1.59286500
H	-6.34207100	2.58864000	-1.66098200
H	-9.39242500	1.51804700	-0.46517400
H	-11.84815600	1.45994000	-0.81599100
H	-13.04829100	-0.71869500	-0.85559700
H	-11.77516900	-2.83310500	-0.54288000
H	-9.31148300	-2.75775200	-0.19516500