Supplementary Material

Magnetochemistry

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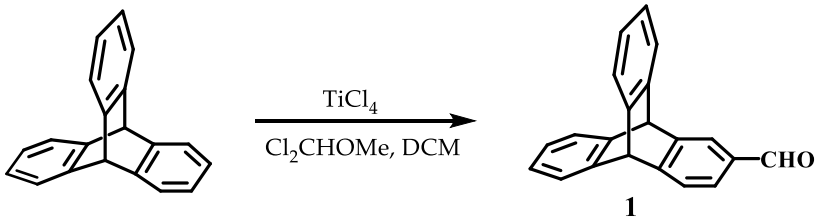
Materials and Methods

The spectroscopic experiments were conducted at room temperature using toluene as the solvent, with UV-vis absorption measurements taken using a CELHXF 300 spectrophotometer. Continuous wave (CW) X-band EPR spectra were recorded in degassed toluene with the concentration of 10^{-4} M unless otherwise stated. CW-EPR measurement were performed on a CIQTEK EPR200-Plus spectrometer using CW4102CR highly sensitive EPR cavity. CIQTEK VTS-L-W2-GDC cryogenic system was used for temperature control. Corrections for g-factors were obtained using 2,2-diphenyl-1-picrylhydrazyl (with a g factor of 2.0037) as the standard, coupled with a frequency counter and liquid helium flow temperature control, and were simulated using WINEPR SimFonia (298 K) and *EasySpin* [1] in Matlab (100 K). The structures were solved by a direct method and refined by a full-matrix least-squares procedure. Variable-temperature magnetic susceptibility was measured with a Quantum Design MPMS-XL-7 SQUID magnetic susceptibility meter, under an external magnetic field of 1T, within a temperature range of 2−270 K (monoradical) and 2−300 K (diradicals). X-ray crystallographic data were obtained using a Nonius Kappa CCD diffractometer that was equipped with a graphite monochromator and utilizing Cu Kα radiation (λ = 1.54184 Å). The structures were solved by a direct method and refined by a full-matrix least-squares procedure. A Teflon tape, weighing approximately 10 mg, was used to wrap the sample prior to measurement in a measuring tube. The background signal from the sample holder was subtracted, and a diamagnetic correction was applied. NMR spectra were obtained using 600 MHz Bruker spectrometers, with ^{1}H NMR recorded using $CDCl_3$ and ^{13}C NMR spectra. Chemical shifts (δ) were reported in parts per million (ppm) relative to TMS at 0 ppm.

The fitting of IT (I, the double integral of the EPR signal) vs. T used the modified Bleaney-Bowers [2] Equation (S1).

$$\boldsymbol{IT} = \frac{\boldsymbol{C}}{\boldsymbol{3} + \boldsymbol{exp}(-\boldsymbol{2J} / \boldsymbol{k_B T})} \quad \text{(S1)}$$

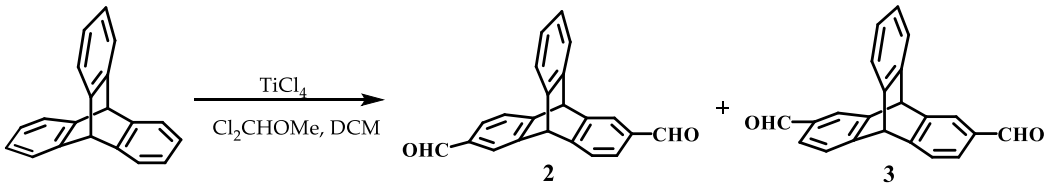
Synthetic procedures



2-Formyltriptycene (1)

To a solution of triptycene [3] (1.27 g, 5 mmol) in dry CH_2Cl_2 (40 mL) was added $TiCl_4$ (2.73 mL, 25 mmol), and the mixture was cooled to 0 °C under an argon atmosphere under stirring 20 min. Then, Cl_2CHOMe (1.81 mL, 25 mmol) in 30 mL of dry CH_2Cl_2 were added dropwise over 30 min at 0 °C. The dark green mixture was stirred for 1 h at 0 °C. The reaction was monitored by TLC. After completion, quenched with ice water (200 g), and stirred for an additional hour. The organic layer was separated and the aqueous layer was extracted three times with 20 mL of CH_2Cl_2. The combined organic fractions were washed consecutively with saturated sodium bicarbonate (50 mL), water (50 mL), brine (50 mL), dried over anhydrous sodium sulphate, and the solvent was evaporated. The residue was purified by chromatography (petroleum ether/CH_2Cl_2 = 1:1, R_f = 0.3) to give the product (0.987 g, yield: 70%) as a pale-yellow solid, ^{1}H NMR (600 MHz, Chloroform-d) δ 9.90 (s, 1H), 7.89 (s, 1H), 7.54 (s, 2H), 7.42 (dt, J = 6.7, 2.7 Hz, 4H), 7.05 – 7.01 (m, 4H), 5.52 (d, J = 9.5 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-d) δ 191.78, 152.11, 146.36, 144.45, 143.85, 129.17, 125.65, 125.57, 125.55, 124.12, 123.94, 123.92, 123.87, 123.85, 123.29, 77.24, 77.22, 77.03, 77.01, 76.98, 76.81, 76.80.

2,6-Diformyltriptycene and 2,7-Diformyltriptycene (2 and 3)



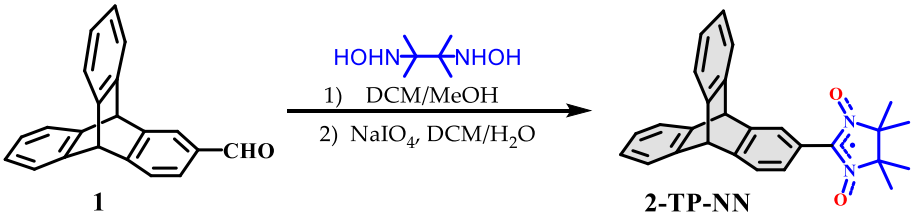
To a solution of triptycene [3] (1.27g, 5 mmol) in dry CH_2Cl_2 (40 mL) was added $TiCl_4$ (8.2 ml, 50 mmol), and the mixture was cooled to 0 °C under an argon atmosphere. under stirring 20 min. Then, Cl_2CHOMe (4.53 ml, 50 mmol) in 30 mL of dry CH_2Cl_2 were added dropwise over 30 min at 0 °C. The dark green mixture was stirred for 1 h at 0 °C. The temperature was allowed to reach RT and the mixture was stirred for an additional 5 hours. The reaction was

monitored by TLC. After completion, quenched with ice water (200 g), and stirred for an additional hour. The organic layer was separated and the aqueous layer was extracted three times with 20 mL of CH_2Cl_2. The combined organic fractions were washed consecutively with saturated sodium bicarbonate (50 mL), water (50 mL), brine (50 mL), dried over anhydrous sodium sulphate, and the solvent was evaporated. The residue was purified by chromatography (petroleum ether/CH_2Cl_2 = 1:50) to give 2,6-diformyltriptycene (605 mg, yield: 39%) as a pale yellow solid and 2,7-diformyltriptycene (540 mg, 35% yield) as a yellow solid.

2,6-Diformyltriptycene (**2**). R_f = 0.5 (petroleum ether/CH_2Cl_2 = 1:50); ^{1}H NMR (600 MHz, Chloroform-d) δ 9.91 (d, J = 0.8 Hz, 2H), 7.92 (s, 2H), 7.58 (d, J = 1.2 Hz, 4H), 7.45 (dd, J = 5.4, 3.2 Hz, 2H), 7.10 - 7.04 (m, 2H), 5.62 (s, 2H). ^{13}C NMR (151 MHz, Chloroform-d) δ 191.60, 151.16, 145.05, 143.12, 134.28, 129.62, 126.08, 124.39, 124.18, 123.53, 77.23, 77.02, 76.80.

2,7-Diformyltriptycene (**3**). R_f = 0.45 (petroleum ether/CH_2Cl_2 = 1:50); ^{1}H NMR (600 MHz, Chloroform-d) δ 9.91 (s, 2H), 7.92 (s, 2H), 7.58 (d, J = 1.8 Hz, 4H), 7.45 (ddd, J = 7.0, 4.9, 2.4 Hz, 2H), 7.09 – 7.03 (m, 2H), 5.63 (s, 1H), 5.60 (s, 1H). ^{13}C NMR (151 MHz, Chloroform-d) δ 191.58, 150.61, 145.61, 143.72, 142.57, 134.33, 129.28, 126.16, 125.99, 124.47, 124.24, 124.11, 123.65, 77.24, 77.02, 76.81.

2-TP-NN

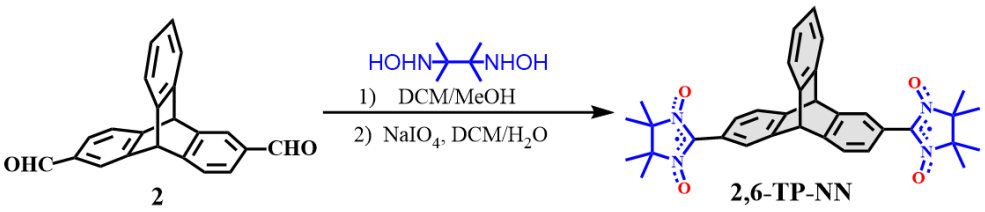


1 **2-TP-NN**

2-formyltriptycene (141 mg, 0.5 mmol) and 2,3- Dimethyl-2,3-bis(hydroxylamino)butane (92 mg, 0.63 mmol) were charged into a flask, evacuated and kept under argon [4]. Mixed solvent with DCM (25 mL) and methanol (5 mL) were added into the flask from syringes and was kept argon bubbling for 15 min. Then the system was heated to 65 °C and refluxed for 48 hours. The color of the reaction mixture turned pale yellow. Then the solvent was evaporated and the white with a solid does not need further purification for synthesis of next step. The Compound was dissolved in 20 mL DCM and charged into a flask. Then the solution was slowly added with 1.1 equiv $NaIO_4$ solved in mixture of 10 mL distilled water and 10 mL DCM. The reaction was kept in ice bath for about 30 min. When the color of mixture turned from pale

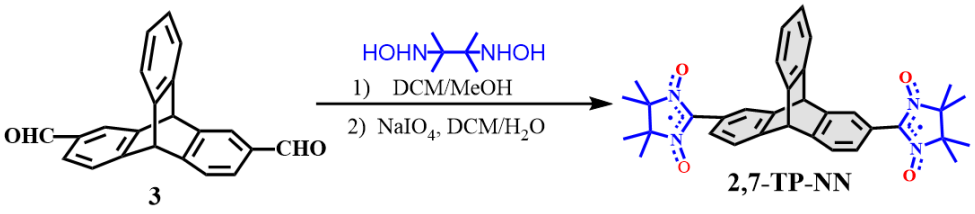
yellow to dark blue, the proceeding of reaction could be stopped and a flesh column was used to purification. A blue sticky solid was separated and collected. DCM as eluent to obtain purple solid powder product (40 mg) in 21% yield two steps.

2,6-TP-NN



2,6-Diformyltriptycene (155 mg, 0.5 mmol) and 2,3-Dimethyl-2,3-bis(hydroxylamino)butane [4] (92 mg, 0.63 mmol) were charged into a flask, evacuated and kept under argon. Mixed solvent with DCM (25 mL) and methanol (5 mL) were added into the flask from syringes and was kept argon bubbling for 15 min. Then the system was heated to 65 °C and refluxed for 48 hours. The color of the reaction mixture turned pale yellow. Then the solvent was evaporated and the white with a solid does not need further purification for synthesis of next step. The Compound was dissolved in 20 mL DCM and charged into a flask. Then the solution was slowly added with 1.1 equiv $NaIO_4$ solved in mixture of 10 mL distilled water and 10 mL DCM. The reaction was kept in ice bath for about 30 min. When the color of mixture turned from pale yellow to dark blue, the proceeding of reaction could be stopped and a flesh column was used to purification. A blue sticky solid was separated and collected. DCM as eluent to obtain blue solid powder product (52 mg) in 18% yield two steps.

2,7-TP-NN



Similar synthetic procedures for 2,7-TP-NN were applied to the substrate of **3** (155 mg) to obtain 2,7-TP-NN (45.9 mg) as a blue solid (16%, two steps).

Optical Properties

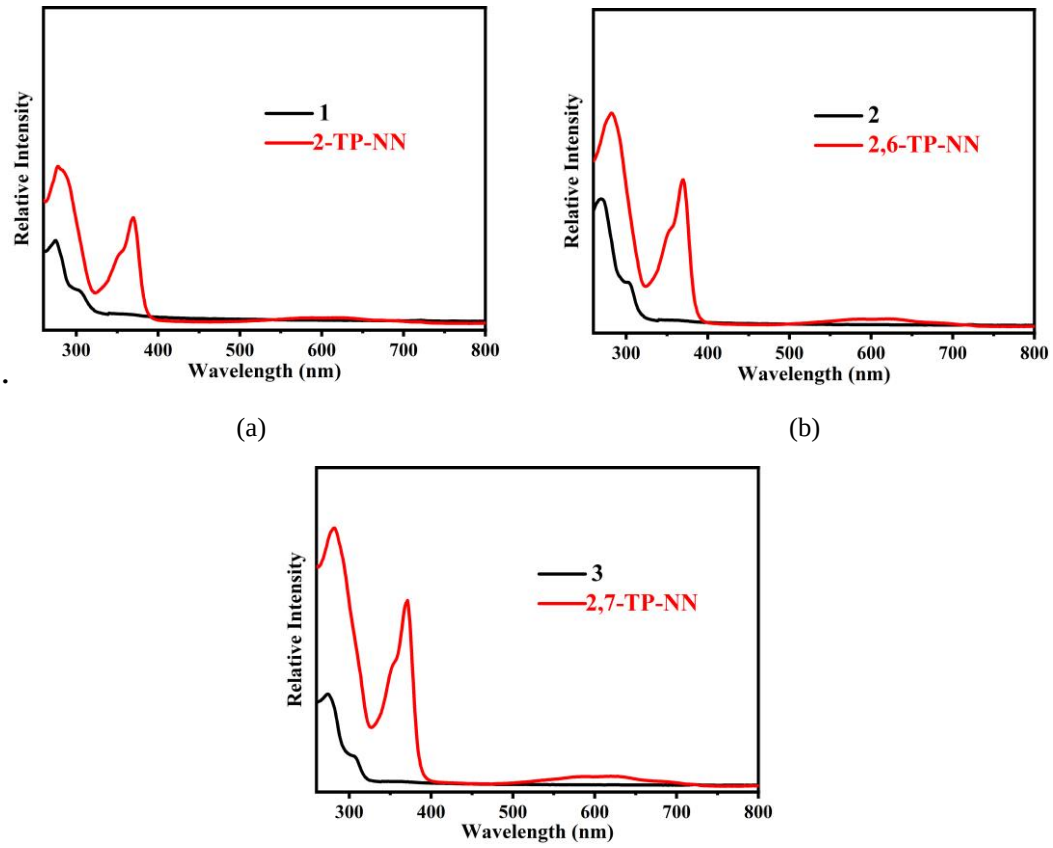
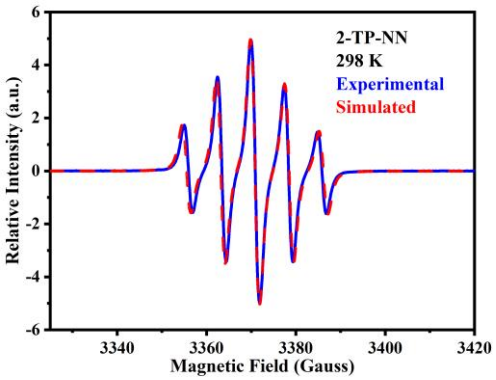
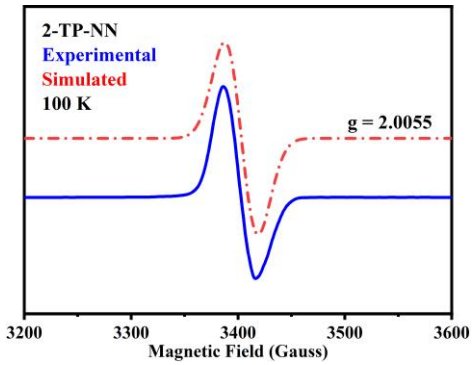


Figure S1. Normalized UV−vis absorption spectra of (a) 2-TP-NN, 7 (b) 2,6-TP-NN, and (c) 2,7-TP-NN in toluene.

EPR spectra

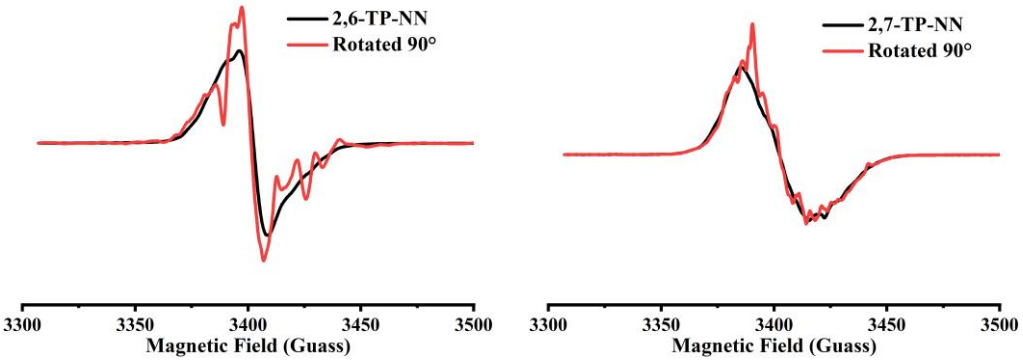


(a)



(b)

Figure S2. EPR spectra in degassed toluene (10^{-4} M) solution for 2-TP-NN at room temperature (bule) and simulated (red) (a). Experimental EPR spectra recorded in toluene solution for 2-TP-NN at 100 K (blue) and simulated (red) (b).



(a) (b)

Figure S3. EPR frozen state ZFS spectra for testing, and then rotated 90° for testing of diradicals 2,6-TP-NN (a) and 2,7-TP-NN (b) at 100 K.

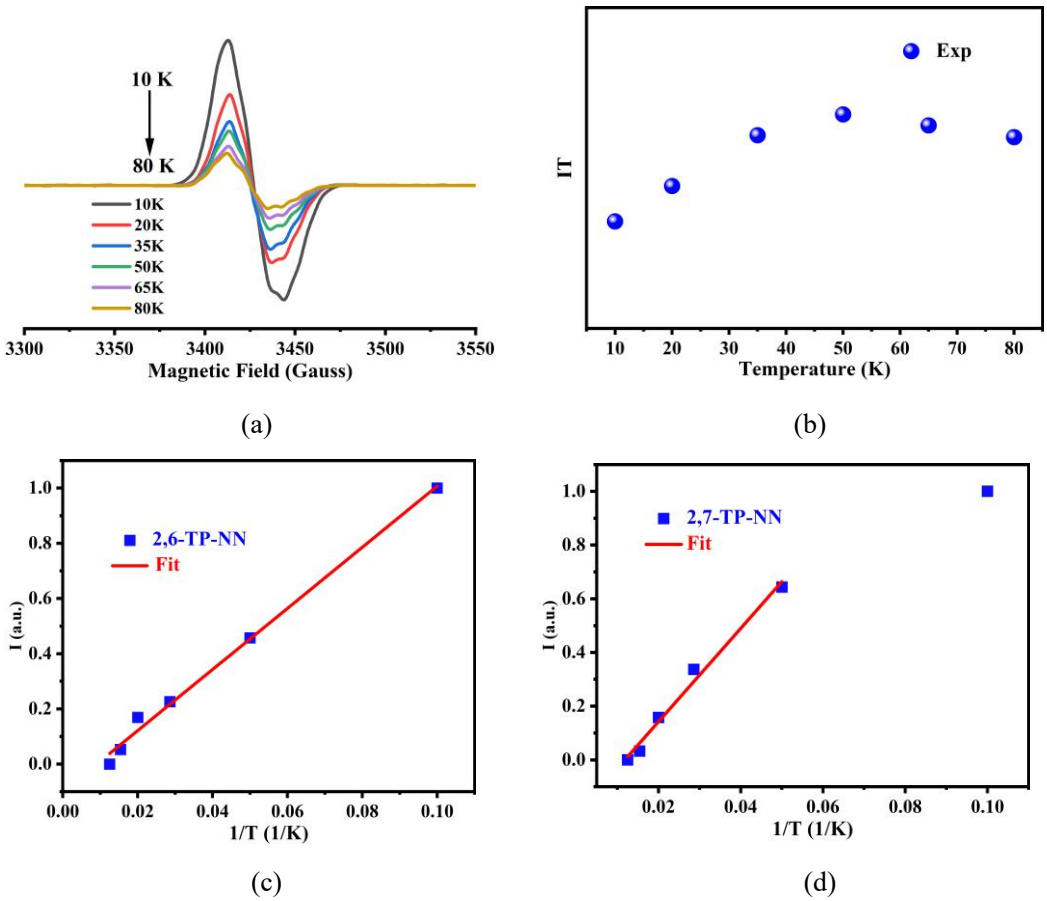
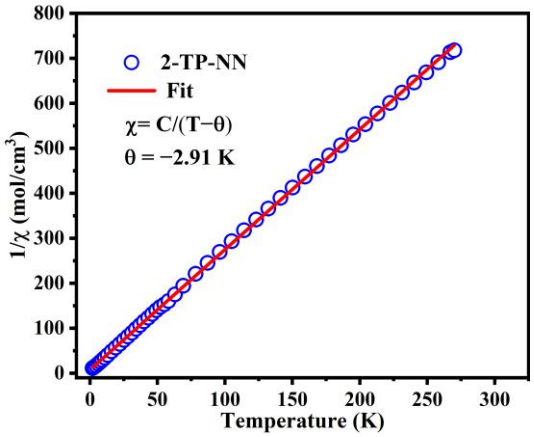
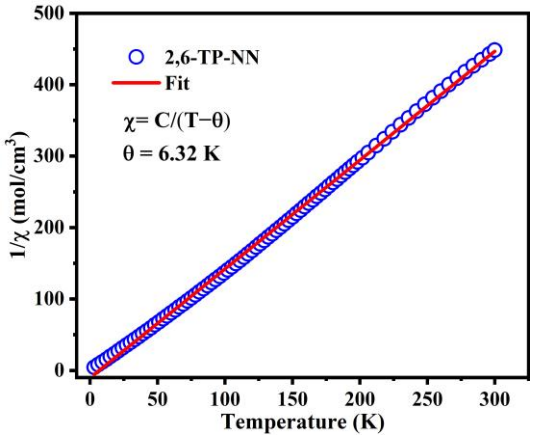


Figure S4. VT-EPR spectra of (a) 2,6-TP-NN and (b) IT−T plot of 2,6-TP-NN. The observed normalized I–T curve presented as a straight line for (c) 2,6-TP-NN and (d) 2,7-TP-NN.

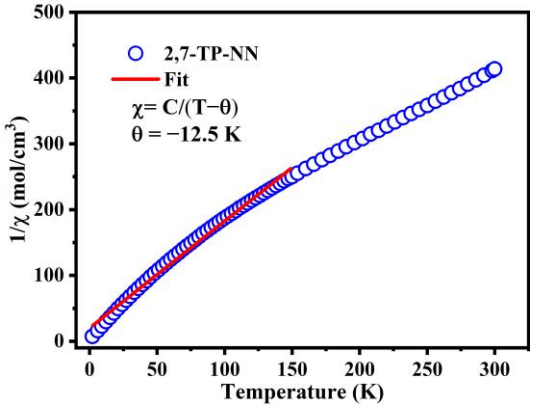
Magnetic Properties



(a)



(b)



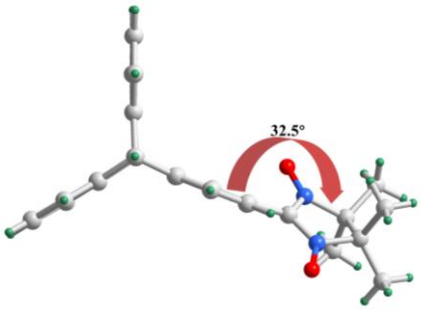
(c)

Figure S5. Curie–Weiss model straight line of (a) 2-TP-NN, (b) 2,6-TP-NN and (c) 2,7-TP-NN.

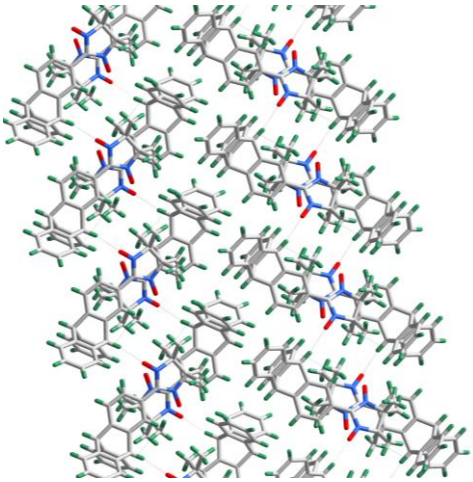
Table S1. Magnetic Properties of 2-TP-NN.

Radicals	T_{max} (K)	θ (K)	J_{exp} (cm^{-1})
2-TP-NN	-	−0.86	−0.75

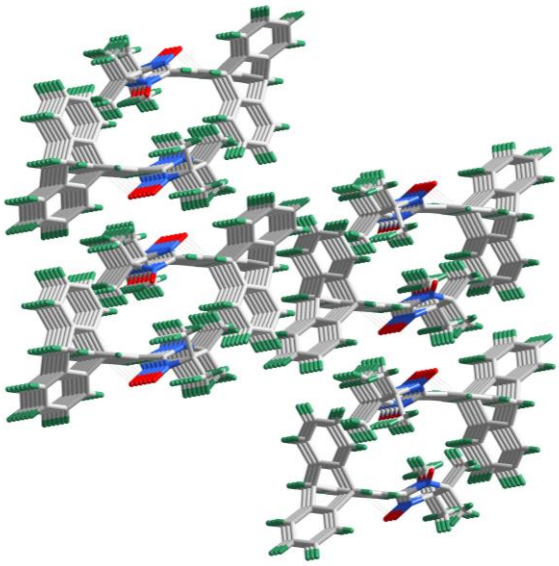
X-ray Crystallography



(a)



(b)



(c)

Figure S6. Single-crystal structures of 2-TP-NN. (a) The benzene ring connected with NN unit with torsions of 32.5°, (b) The crystal packing of 2-TP-NN along axis b and (c) axis a.

Table S2. Crystal data and structure refinement for 2-TP-NN.

Identification code	2-TP-NN
Empirical formula	$C_{27}H_{25}N_2O_2$
Formula weight	409.49
Temperature/K	291
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9820(4)
b/Å	8.1768(3)
c/Å	26.9862(9)
α/°	90
β/°	99.809(4)
γ/°	90
Volume/Å^3	2170.43(14)
Z	4
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	0.626
F(000)	868.0
Crystal size/mm^3	0.25 × 0.23 × 0.22
Radiation	Cu Kα (λ = 1.54184)
2ϴ range for data collection/°	9.04 to 139.826
Index ranges	$-12 \le h \le 11$, $-9 \le k \le 9$, $-28 \le l \le 32$
Reflections collected	16734
Independent reflections	4062 [R_{int} = 0.0385, R_{sigma} = 0.0261]
Data/restraints/parameters	4062/0/284
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0568, wR_2 = 0.1563
Final R indexes [all data]	R_1 = 0.0738, wR_2 = 0.1708
Largest diff. peak/hole / e Å-3	0.19/−0.32

Table S3. Bond Lengths for 2-TP-NN.

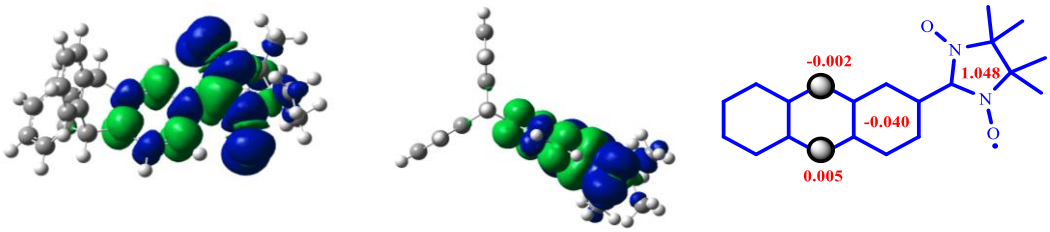
Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	O1	1.279(3)	C1	C21	1.465(3)
N1	C21	1.339(3)	C1	C6	1.384(3)
N1	C22	1.511(3)	C15	C14	1.516(3)
O2	N2	1.283(3)	C15	C16	1.379(3)
N2	C21	1.342(3)	C13	C14	1.519(3)
N2	C23	1.496(3)	C13	C12	1.384(3)
C3	C7	1.533(3)	C9	C10	1.389(3)
C3	C4	1.394(3)	C5	C6	1.377(3)
C3	C2	1.377(3)	C12	C11	1.386(4)
C7	C20	1.518(3)	C19	C18	1.386(4)
C7	C8	1.520(3)	C16	C17	1.383(4)
C20	C15	1.404(3)	C11	C10	1.378(4)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C20	C19	1.380(3)	C22	C23	1.541(4)
C8	C13	1.401(3)	C22	C27	1.509(4)
C8	C9	1.381(3)	C22	C26	1.526(4)
C4	C14	1.520(3)	C23	C25	1.535(4)
C4	C5	1.381(3)	C23	C24	1.523(4)
C1	C2	1.403(3)	C17	C18	1.370(4)

Table S4. Bond Angles for 2-TP-NN.

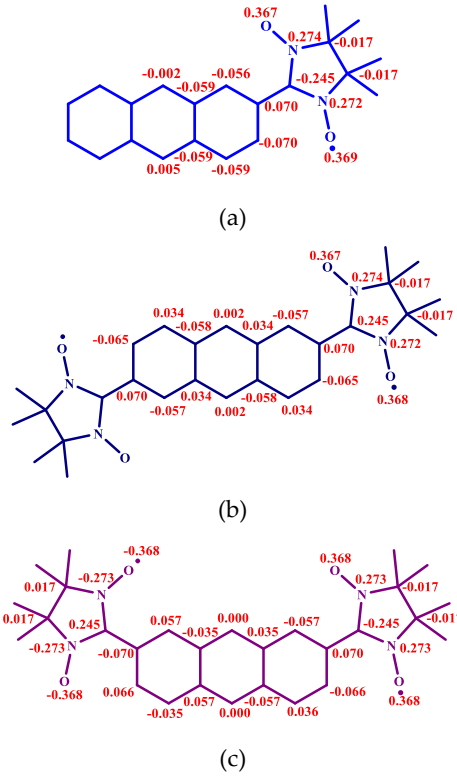
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	N1	C21	126.84(19)	C3	C2	C1	119.07(19)
O1	N1	C22	121.61(18)	C15	C14	C4	104.19(17)
C21	N1	C22	111.32(18)	C15	C14	C13	106.09(17)
O2	N2	C21	127.12(19)	C13	C14	C4	107.00(17)
O2	N2	C23	121.19(19)	C8	C9	C10	119.0(2)
C21	N2	C23	111.37(18)	C6	C5	C4	119.42(19)
C4	C3	C7	112.77(17)	N1	C21	N2	108.76(18)
C2	C3	C7	126.45(18)	N1	C21	C1	125.97(19)
C2	C3	C4	120.62(18)	N2	C21	C1	125.08(19)
C20	C7	C3	104.15(17)	C5	C6	C1	121.0(2)
C20	C7	C8	105.96(16)	C13	C12	C11	119.2(2)
C8	C7	C3	106.88(16)	C20	C19	C18	119.1(2)
C15	C20	C7	112.88(18)	C15	C16	C17	119.0(3)
C19	C20	C7	127.2(2)	C10	C11	C12	120.6(2)
C19	C20	C15	119.9(2)	C11	C10	C9	120.6(2)
C13	C8	C7	112.96(18)	N1	C22	C23	100.09(17)
C9	C8	C7	126.57(19)	N1	C22	C26	105.6(2)
C9	C8	C13	120.40(19)	C27	C22	N1	109.9(2)
C3	C4	C14	113.28(17)	C27	C22	C23	115.8(2)
C5	C4	C3	120.16(18)	C27	C22	C26	110.5(2)
C5	C4	C14	126.35(18)	C26	C22	C23	114.0(2)
C2	C1	C21	121.47(19)	N2	C23	C22	100.25(18)
C6	C1	C2	119.74(19)	N2	C23	C25	105.0(2)
C6	C1	C21	118.65(19)	N2	C23	C24	110.7(2)
C20	C15	C14	113.08(19)	C25	C23	C22	113.7(2)
C16	C15	C20	120.4(2)	C24	C23	C22	115.9(2)
C16	C15	C14	126.5(2)	C24	C23	C25	110.4(2)
C8	C13	C14	113.04(18)	C18	C17	C16	120.8(3)
C12	C13	C8	120.1(2)	C17	C18	C19	120.8(3)
C12	C13	C14	126.9(2)				

Computational Studies



(a) (b) (c)

Figure S7. Spin density distributions and spin population of 2-TP-NN were calculated using UB3LYP/6-31G method (blue and green surfaces correspond to α and β spin densities, respectively, with an isovalue of 0.004.).



(a)

(b)

(c)

Figure S8. Atomic spin populations calculated using Mulliken protocol at the UB3LYP/6-31G level. (a) 2-TP-NN, (b) 2,6-TP-NN and (c) 2,7-TP-NN.

Table S5. Summary of diradical calculation results [5].

Radicals	E_{BS}-E_T **(eV)**	$\langle S^2 \rangle_{BS}$	$\langle S^2 \rangle_T$	J_{calc} **(cm^{-1})**
2,6-TP-NN	0.00013	1.141213	2.141606	1.06
2,7-TP-NN	−0.00043	1.142336	2.141535	−3.50

Table S6. HOMO, LUMO and HOMO−LUMO(ΔE_{HL}) energy.

Radicals	HOMO (eV)	LUMO (eV)	ΔE_{HL} (eV)
2-TP-NN	−5.29	−1.36	3.93
2,6-TP-NN	−5.27	−1.36	3.91
2,7-TP-NN	−5.27	−2.24	3.03

The spatial distribution of molecular orbitals (red and blue color represent the different phase of the orbital coefficients), the isovalue is 0.004.

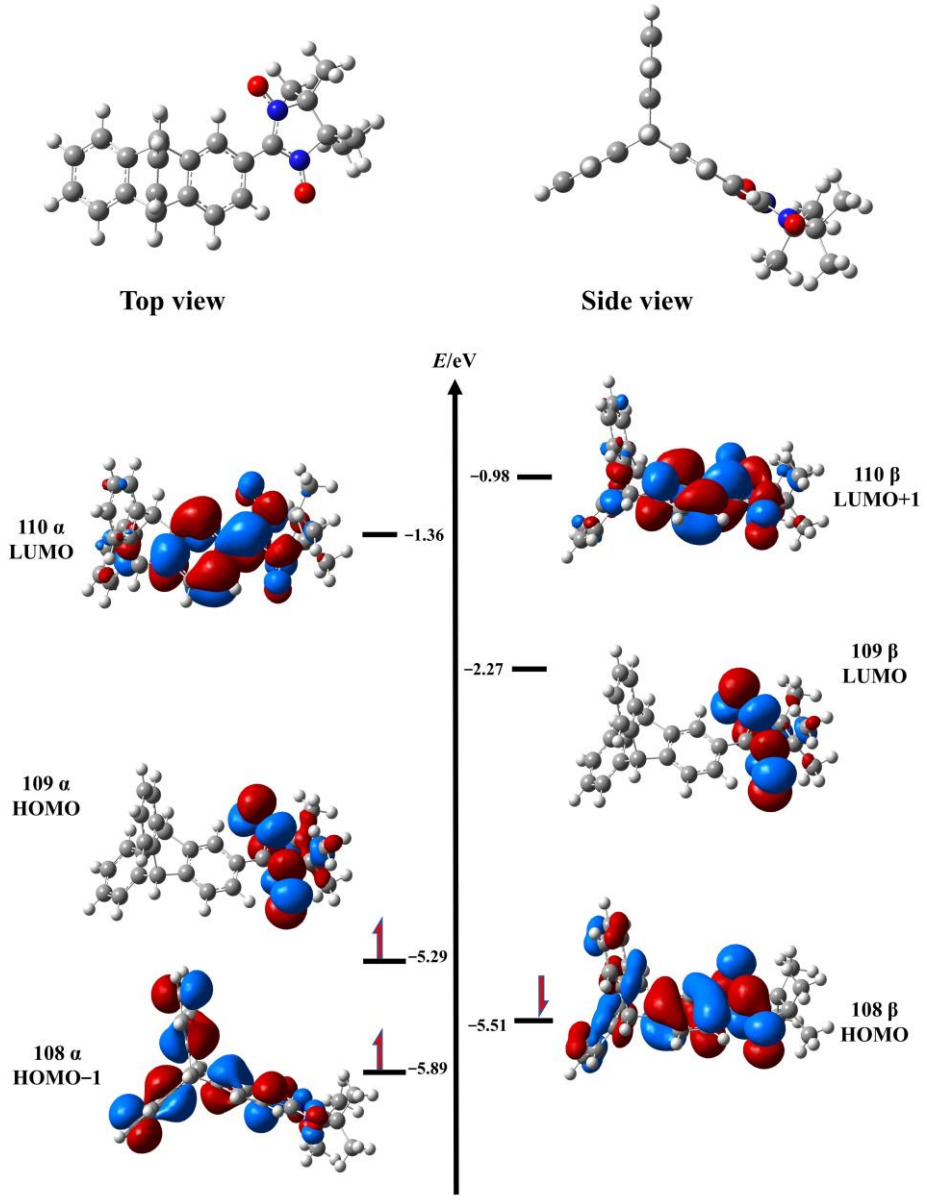


Figure S9. The 2-TP-NN spatial distribution of molecular orbitals.

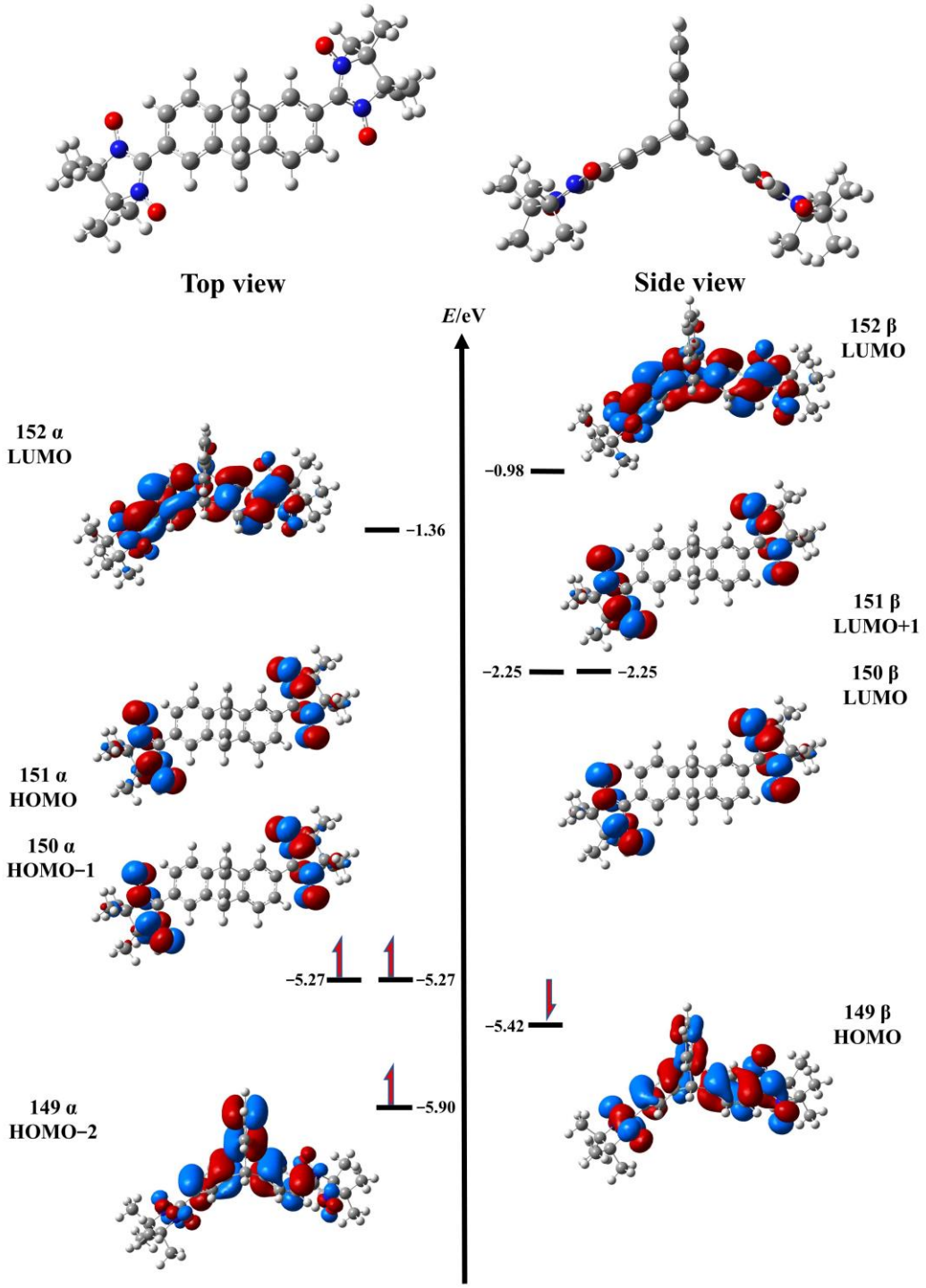


Figure S10. The 2,6-TP-NN spatial distribution of molecular orbitals.

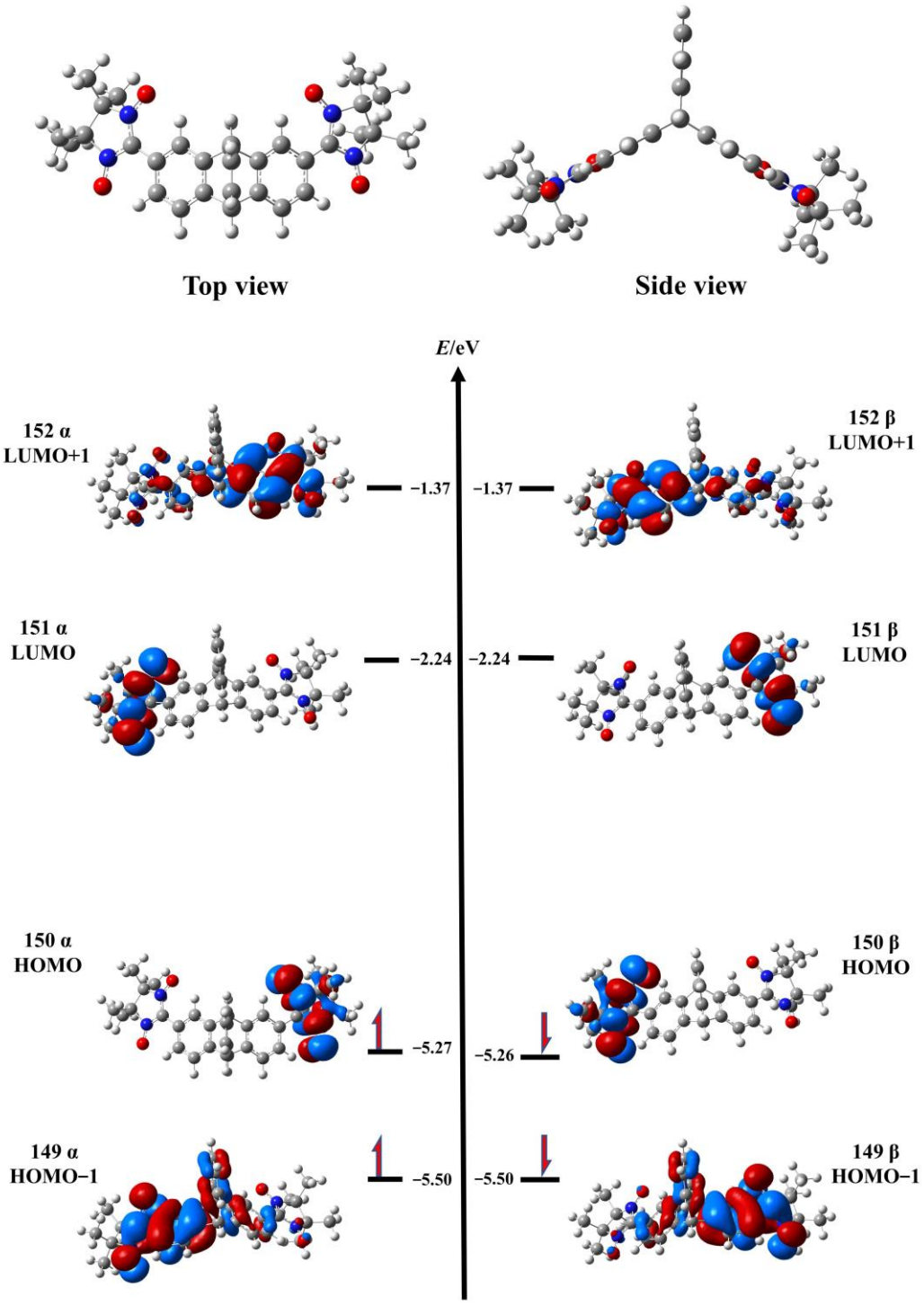


Figure S11. The 2,7-TP-NN spatial distribution of molecular orbitals.

References

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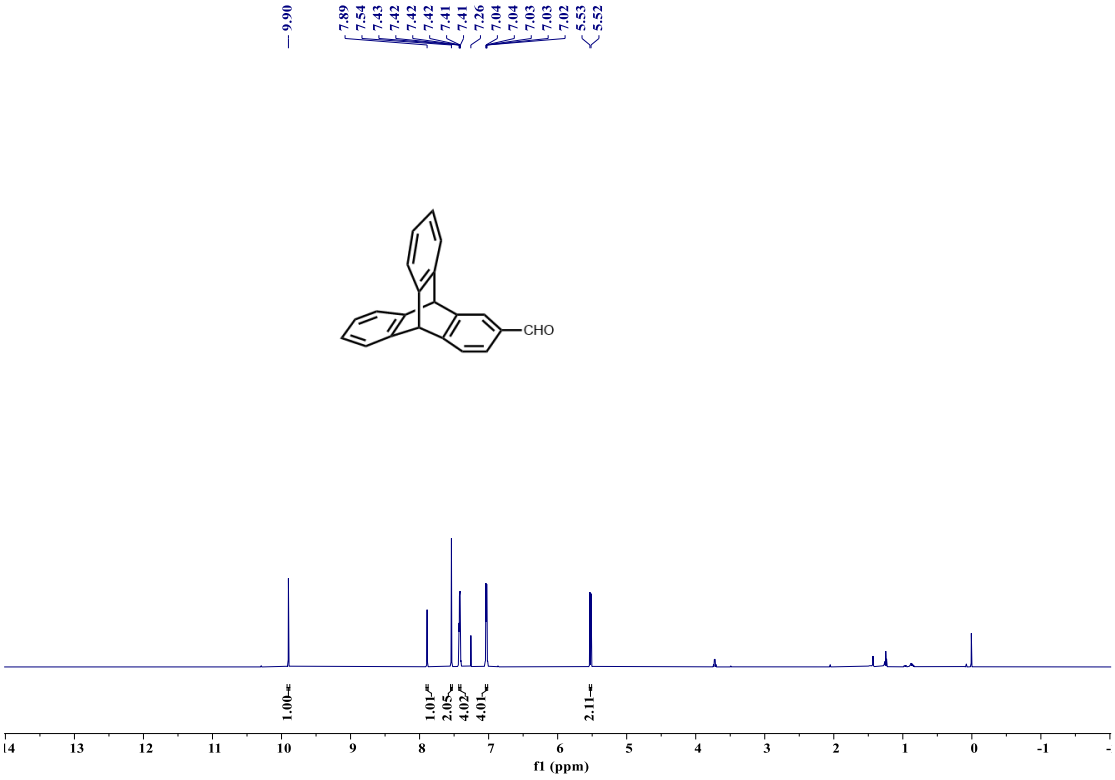
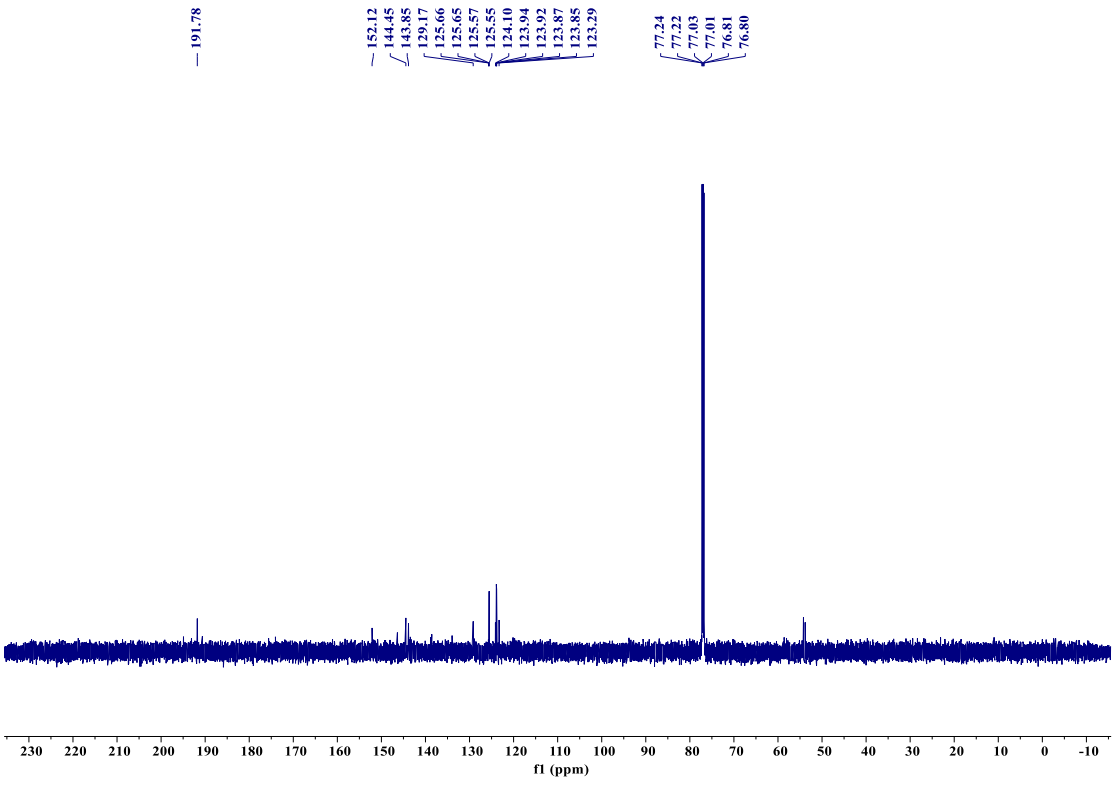
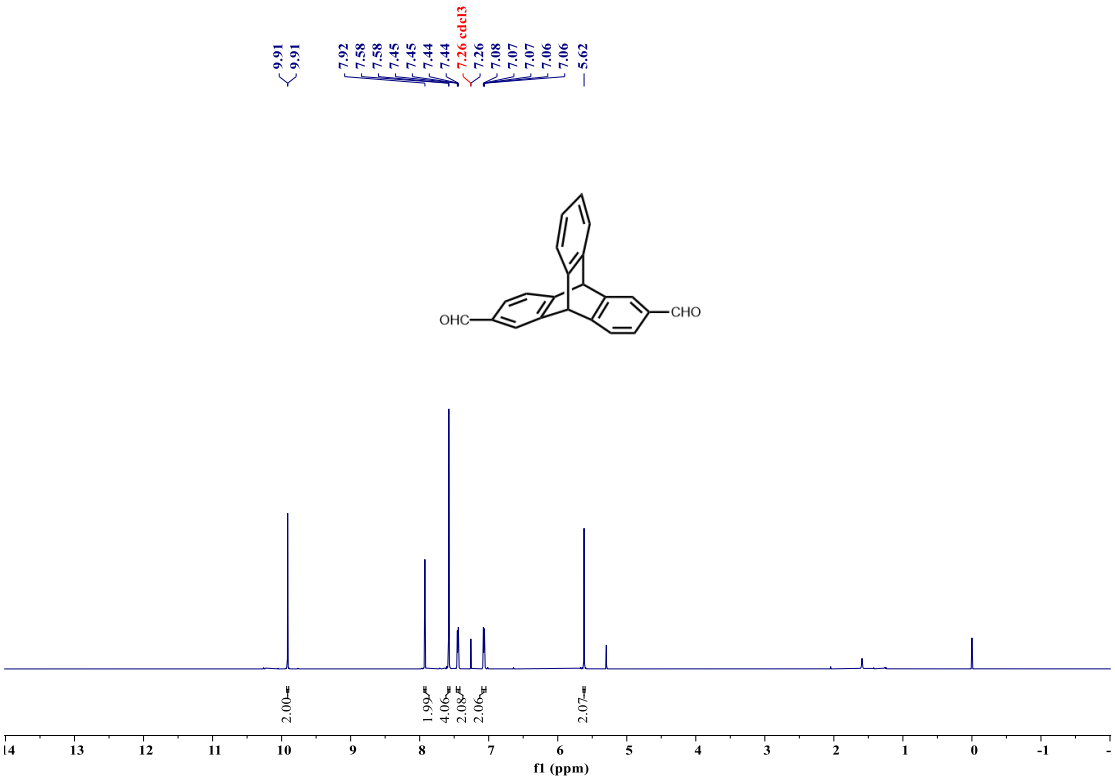
Copies of ^{1}H, ^{13}C NMR Spectra Mass Spectra



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7.07
7.07
7.06
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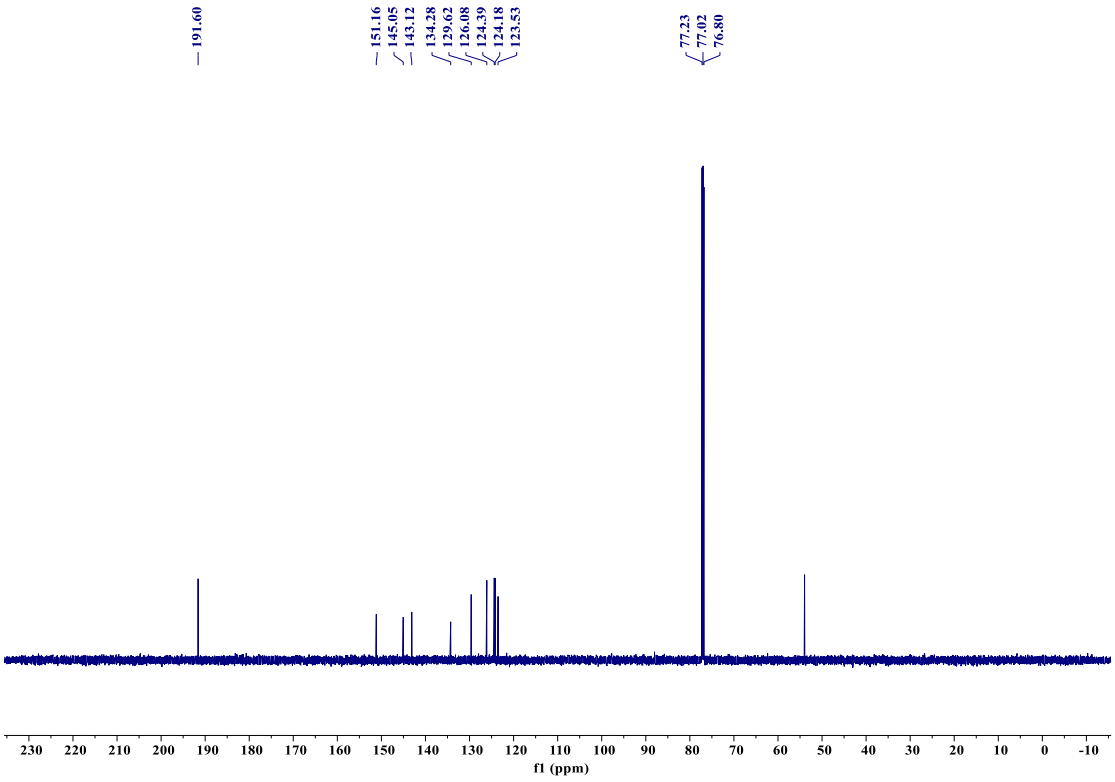
OHC
CHO
2.00
1.99
4.06
2.08
2.06
2.07
f1 (ppm)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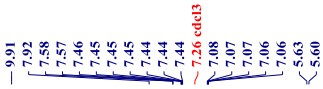
f1 (ppm)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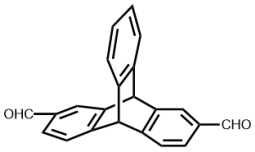
7.07
7.07
7.06
7.06
5.63
5.60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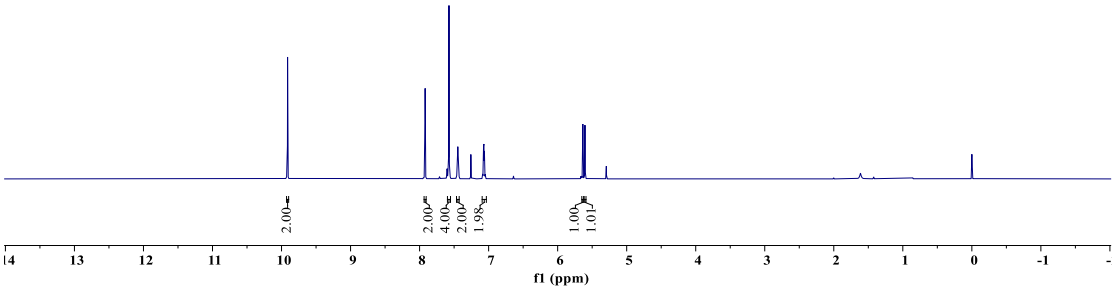
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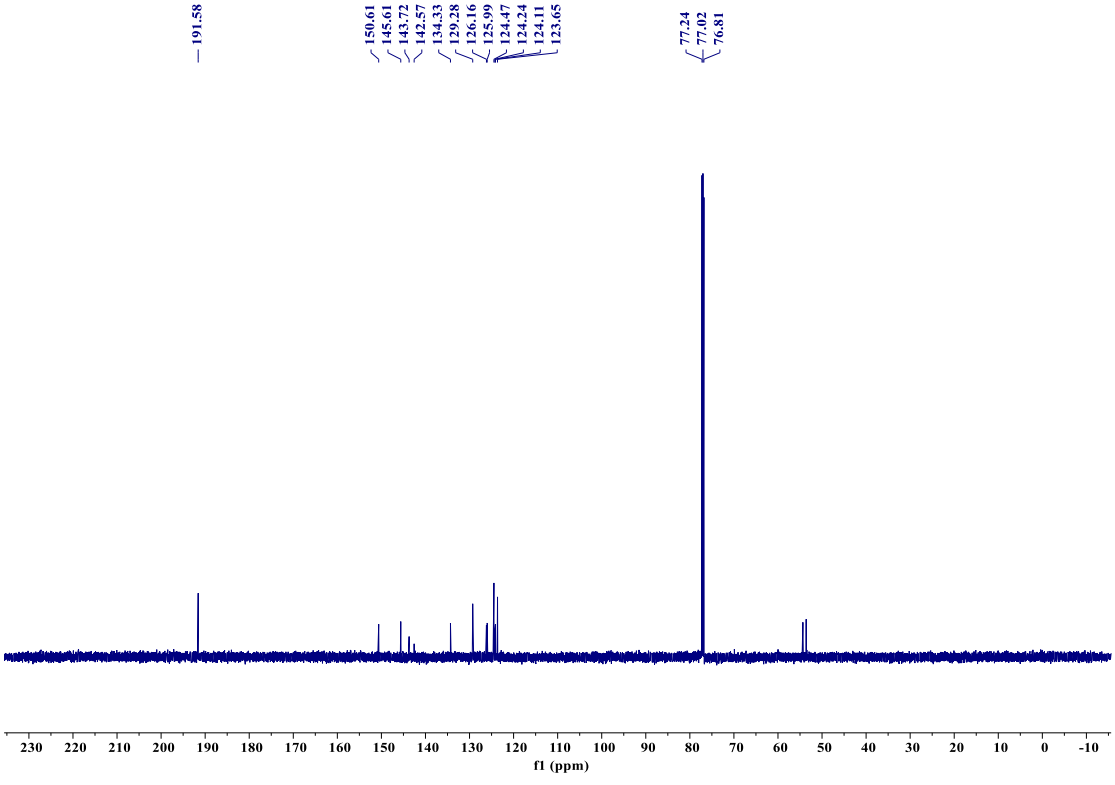
5
4
3
2
1
0
-1
f1 (ppm)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200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Geometry Coordinates

2-PT-NN (double**)**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 2

C	2.37	-1.078	2.542
C	3.593	-0.85	1.672
C	3.451	-1.243	0.391
C	2.096	-1.842	0.06
C	2.068	-2.555	2.365
C	1.926	-2.949	1.085
C	1.107	-0.78	0.506
C	1.253	-0.387	1.783
C	0.432	0.544	2.28
C	-0.521	1.073	1.495
C	-0.693	0.706	0.205
C	0.149	-0.242	-0.263
C	4.461	-1.094	-0.478
C	5.615	-0.548	-0.059
C	5.756	-0.156	1.218
C	4.746	-0.305	2.089
C	1.94	-3.441	3.364
C	1.67	-4.724	3.075
C	1.528	-5.117	1.798
C	1.656	-4.231	0.797
C	-1.66	1.244	-0.581
N	-1.87	0.832	-1.77
C	-2.783	1.782	-2.479
C	-3.456	2.424	-1.236
N	-2.415	2.199	-0.187
O	-2.2466	2.82963	0.9555
O	-1.39304	-0.25204	-2.35595
C	-3.765	1.159	-3.487
C	-1.87	2.758	-3.256
C	-3.854	3.898	-1.445
C	-4.718	1.675	-0.75
H	2.484	-0.751	3.596
H	1.983	-2.169	-0.994
H	0.535	0.863	3.33
H	-1.177	1.812	1.983
H	0.105	-0.608	-1.301
H	4.344	-1.416	-1.525
H	6.45	-0.422	-0.768
H	6.707	0.291	1.553
H	4.86	0.017	3.137

H	2.056	-3.117	4.411
H	1.563	-5.459	3.891
H	1.306	-6.173	1.57
H	1.54	-4.552	-0.25
H	-3.216	0.679	-4.329
H	-4.414	0.373	-3.044
H	-4.433	1.937	-3.919
H	-2.456	3.526	-3.808
H	-1.151	3.283	-2.588
H	-1.263	2.209	-4.012
H	-4.337	4.317	-0.533
H	-2.987	4.556	-1.669
H	-4.58	3.997	-2.283
H	-5.566	1.789	-1.462
H	-4.537	0.588	-0.6
H	-5.061	2.078	0.23

2,6-TP-NN (singlet)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.817	1.367	-1.081
C	-3.151	0.074	-0.905
C	-2.233	-0.905	-0.965
C	-0.953	-0.594	-1.205
C	-0.6	0.692	-1.385
C	-1.525	1.66	-1.324
C	0.878	0.908	-1.655
C	0.19	-1.587	-1.306
C	1.566	0.217	-0.493
C	1.212	-1.068	-0.311
C	1.756	-1.783	0.683
C	2.664	-1.234	1.514
C	3.007	0.053	1.315
C	2.468	0.78	0.323
C	1.168	0.001	-2.837
C	0.813	-1.286	-2.657
C	1.019	-2.187	-3.629
C	1.581	-1.793	-4.783
C	1.934	-0.51	-4.963
C	1.729	0.393	-3.99
C	3.257	-2.098	2.621
C	-3.831	2.504	-1.031
N	3.885	-1.315	3.684
C	5.264	-1.786	3.791
C	5.203	-3.21	3.178

N	4.224	-3.062	2.107
N	-5.049	2.152	-0.305
C	-6.167	2.408	-1.212
C	-5.577	3.415	-2.235
N	-4.192	2.976	-2.364
C	-6.578	1.057	-1.85
C	-7.433	2.927	-0.492
C	-5.566	4.869	-1.699
C	-6.312	3.456	-3.591
O	-3.963	2.13	-3.351
O	-5.119	2.721	0.885
C	6.16	-0.811	2.986
C	5.807	-1.75	5.237
C	4.66	-4.265	4.174
C	6.558	-3.747	2.671
O	4.732	-2.788	0.919
O	3.202	-1.306	4.814
H	-4.195	-0.22	-0.712
H	-2.527	-1.957	-0.821
H	-1.214	2.705	-1.482
H	1.172	1.968	-1.802
H	-0.105	-2.646	-1.157
H	1.456	-2.836	0.81
H	3.749	0.549	1.961
H	2.764	1.831	0.175
H	0.729	-3.239	-3.48
H	1.754	-2.528	-5.587
H	2.396	-0.195	-5.914
H	2.019	1.446	-4.136
H	-7.462	1.164	-2.517
H	-5.767	0.583	-2.442
H	-6.86	0.319	-1.064
H	-7.825	2.174	0.229
H	-7.259	3.858	0.089
H	-8.246	3.145	-1.22
H	-6.589	5.304	-1.659
H	-5.125	4.958	-0.682
H	-4.966	5.53	-2.364
H	-5.83	4.183	-4.284
H	-6.319	2.477	-4.118
H	-7.373	3.766	-3.463
H	7.237	-1.08	3.058
H	5.899	-0.756	1.909
H	6.066	0.227	3.38

H	5.82	-0.711	5.637
H	5.207	-2.354	5.951
H	6.85	-2.138	5.282
H	5.395	-4.492	4.979
H	3.711	-3.958	4.664
H	4.451	-5.228	3.655
H	6.445	-4.763	2.228
H	7.019	-3.111	1.885
H	7.295	-3.823	3.502

2,6-TP-NN (triplet)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-2.817	1.367	-1.081
C	-3.151	0.074	-0.905
C	-2.233	-0.905	-0.965
C	-0.953	-0.594	-1.205
C	-0.6	0.692	-1.385
C	-1.525	1.66	-1.324
C	0.878	0.908	-1.655
C	0.19	-1.587	-1.306
C	1.566	0.217	-0.493
C	1.212	-1.068	-0.311
C	1.756	-1.783	0.683
C	2.664	-1.234	1.514
C	3.007	0.053	1.315
C	2.468	0.78	0.323
C	1.168	0.001	-2.837
C	0.813	-1.286	-2.657
C	1.019	-2.187	-3.629
C	1.581	-1.793	-4.783
C	1.934	-0.51	-4.963
C	1.729	0.393	-3.99
C	3.257	-2.098	2.621
C	-3.831	2.504	-1.031
N	3.885	-1.315	3.684
C	5.264	-1.786	3.791
C	5.203	-3.21	3.178
N	4.224	-3.062	2.107
N	-5.049	2.152	-0.305
C	-6.167	2.408	-1.212
C	-5.577	3.415	-2.235
N	-4.192	2.976	-2.364
C	-6.578	1.057	-1.85
C	-7.433	2.927	-0.492

C	-5.566	4.869	-1.699
C	-6.312	3.456	-3.591
O	-3.963	2.13	-3.351
O	-5.119	2.721	0.885
C	6.16	-0.811	2.986
C	5.807	-1.75	5.237
C	4.66	-4.265	4.174
C	6.558	-3.747	2.671
O	4.732	-2.788	0.919
O	3.202	-1.306	4.814
H	-4.195	-0.22	-0.712
H	-2.527	-1.957	-0.821
H	-1.214	2.705	-1.482
H	1.172	1.968	-1.802
H	-0.105	-2.646	-1.157
H	1.456	-2.836	0.81
H	3.749	0.549	1.961
H	2.764	1.831	0.175
H	0.729	-3.239	-3.48
H	1.754	-2.528	-5.587
H	2.396	-0.195	-5.914
H	2.019	1.446	-4.136
H	-7.462	1.164	-2.517
H	-5.767	0.583	-2.442
H	-6.86	0.319	-1.064
H	-7.825	2.174	0.229
H	-7.259	3.858	0.089
H	-8.246	3.145	-1.22
H	-6.589	5.304	-1.659
H	-5.125	4.958	-0.682
H	-4.966	5.53	-2.364
H	-5.83	4.183	-4.284
H	-6.319	2.477	-4.118
H	-7.373	3.766	-3.463
H	7.237	-1.08	3.058
H	5.899	-0.756	1.909
H	6.066	0.227	3.38
H	5.82	-0.711	5.637
H	5.207	-2.354	5.951
H	6.85	-2.138	5.282
H	5.395	-4.492	4.979
H	3.711	-3.958	4.664
H	4.451	-5.228	3.655
H	6.445	-4.763	2.228

H	7.019	-3.111	1.885
H	7.295	-3.823	3.502

2,7-TP-NN (singlet)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.404	1.86	1.399
C	-2.674	0.557	1.183
C	-1.66	-0.324	1.293
C	-0.426	0.083	1.62
C	-0.179	1.388	1.838
C	-1.171	2.28	1.725
C	1.258	1.71	2.203
C	0.781	-0.823	1.781
C	2.066	1.092	1.077
C	1.821	-0.213	0.859
C	2.475	-0.869	-0.11
C	3.382	-0.239	-0.882
C	3.618	1.066	-0.643
C	2.969	1.734	0.324
C	1.54	0.807	3.39
C	1.294	-0.5	3.173
C	1.502	-1.399	4.146
C	1.959	-0.984	5.338
C	2.205	0.319	5.555
C	1.997	1.22	4.582
C	4.1	-1.029	-1.97
C	-4.06	0.042	0.815
N	5.365	-0.424	-2.363
C	5.511	-0.762	-3.774
C	4.046	-0.551	-4.254
N	3.294	-1.194	-3.179
N	-4.915	1.081	0.256
C	-6.262	0.717	0.681
C	-5.973	0.254	2.137
N	-4.767	-0.55	1.95
C	-7.201	1.933	0.569
C	-6.852	-0.419	-0.188
C	-7.085	-0.613	2.76
C	-5.735	1.449	3.092
O	-4.06	-0.728	3.051
O	-4.756	1.269	-1.042
C	6.546	0.167	-4.434
C	5.986	-2.221	-3.981
C	3.714	-1.23	-5.598

C	3.692	0.948	-4.401
O	2.033	-0.811	-3.096
O	6.388	-0.749	-1.594
H	-3.193	2.623	1.315
H	-1.839	-1.398	1.123
H	-0.973	3.35	1.901
H	1.46	2.786	2.381
H	0.578	-1.899	1.602
H	2.257	-1.937	-0.272
H	4.355	1.627	-1.239
H	3.175	2.802	0.502
H	1.3	-2.467	3.966
H	2.133	-1.717	6.143
H	2.58	0.651	6.538
H	2.197	2.289	4.759
H	-8.176	1.735	1.068
H	-6.761	2.85	1.019
H	-7.415	2.182	-0.495
H	-6.91	-0.129	-1.261
H	-6.261	-1.36	-0.139
H	-7.894	-0.661	0.12
H	-8.06	-0.077	2.765
H	-7.224	-1.576	2.22
H	-6.842	-0.883	3.813
H	-5.425	1.116	4.108
H	-4.949	2.144	2.728
H	-6.665	2.04	3.242
H	6.538	0.058	-5.542
H	6.371	1.238	-4.19
H	7.577	-0.065	-4.081
H	6.978	-2.405	-3.511
H	5.284	-2.974	-3.562
H	6.117	-2.451	-5.062
H	4.39	-0.876	-6.408
H	3.792	-2.338	-5.544
H	2.668	-1.011	-5.912
H	2.616	1.101	-4.643
H	3.901	1.535	-3.482
H	4.256	1.418	-5.237

2,7-TP-NN (triplet)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-2.404	1.86	1.399
C	-2.674	0.557	1.183

C	-1.66	-0.324	1.293
C	-0.426	0.083	1.62
C	-0.179	1.388	1.838
C	-1.171	2.28	1.725
C	1.258	1.71	2.203
C	0.781	-0.823	1.781
C	2.066	1.092	1.077
C	1.821	-0.213	0.859
C	2.475	-0.869	-0.11
C	3.382	-0.239	-0.882
C	3.618	1.066	-0.643
C	2.969	1.734	0.324
C	1.54	0.807	3.39
C	1.294	-0.5	3.173
C	1.502	-1.399	4.146
C	1.959	-0.984	5.338
C	2.205	0.319	5.555
C	1.997	1.22	4.582
C	4.1	-1.029	-1.97
C	-4.06	0.042	0.815
N	5.365	-0.424	-2.363
C	5.511	-0.762	-3.774
C	4.046	-0.551	-4.254
N	3.294	-1.194	-3.179
N	-4.915	1.081	0.256
C	-6.262	0.717	0.681
C	-5.973	0.254	2.137
N	-4.767	-0.55	1.95
C	-7.201	1.933	0.569
C	-6.852	-0.419	-0.188
C	-7.085	-0.613	2.76
C	-5.735	1.449	3.092
O	-4.06	-0.728	3.051
O	-4.756	1.269	-1.042
C	6.546	0.167	-4.434
C	5.986	-2.221	-3.981
C	3.714	-1.23	-5.598
C	3.692	0.948	-4.401
O	2.033	-0.811	-3.096
O	6.388	-0.749	-1.594
H	-3.193	2.623	1.315
H	-1.839	-1.398	1.123
H	-0.973	3.35	1.901
H	1.46	2.786	2.381

H	0.578	-1.899	1.602
H	2.257	-1.937	-0.272
H	4.355	1.627	-1.239
H	3.175	2.802	0.502
H	1.3	-2.467	3.966
H	2.133	-1.717	6.143
H	2.58	0.651	6.538
H	2.197	2.289	4.759
H	-8.176	1.735	1.068
H	-6.761	2.85	1.019
H	-7.415	2.182	-0.495
H	-6.91	-0.129	-1.261
H	-6.261	-1.36	-0.139
H	-7.894	-0.661	0.12
H	-8.06	-0.077	2.765
H	-7.224	-1.576	2.22
H	-6.842	-0.883	3.813
H	-5.425	1.116	4.108
H	-4.949	2.144	2.728
H	-6.665	2.04	3.242
H	6.538	0.058	-5.542
H	6.371	1.238	-4.19
H	7.577	-0.065	-4.081
H	6.978	-2.405	-3.511
H	5.284	-2.974	-3.562
H	6.117	-2.451	-5.062
H	4.39	-0.876	-6.408
H	3.792	-2.338	-5.544
H	2.668	-1.011	-5.912
H	2.616	1.101	-4.643
H	3.901	1.535	-3.482
H	4.256	1.418	-5.237