Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Reversible mechanochromism and aggregation induced enhanced emission in phenothiazine substituted tetraphenylethylene

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Experimental section

Synthesis of 10-propyl-10H-phenothiazine (2)

Phenothiazine (5.0g, 25.1mmol) and propyl iodide (5.5g, 3.18mL, 32.6mmol) were dissolved in 50mL DMSO and stirred for 30min at room temperature. Sodium hydroxide (2.8g, 50mmol) was slowly added and stirred for overnight at room temperature. The reaction mixture was poured into water and extracted with dichloromethane. The organic layer was separated and dried over anhydrous sodium sulfate. The product was purified using column chromatography with hexane. The product was obtained as white solid. Yield: 5.9g (97%).

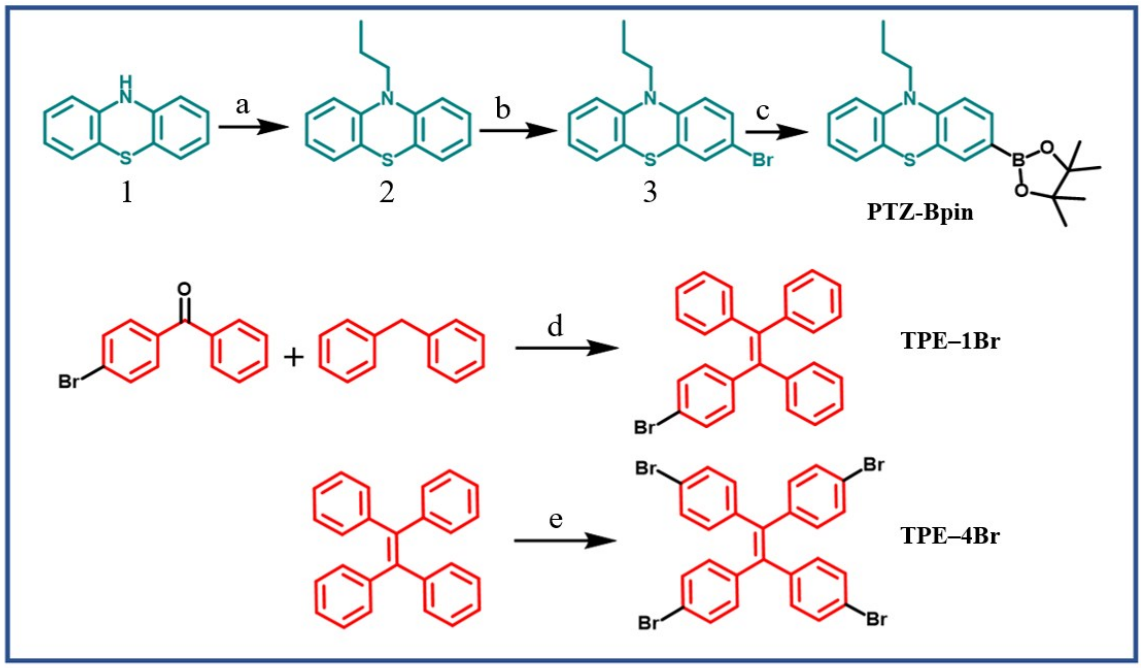
Synthesis of 3-bromo-10-propyl-10H-phenothiazine (3)

To a solution of compound 10-propyl-10H-phenothiazine (1.32g, 5.8mmol) in 10mL chloroform, a solution of NaOH (0.26g, 6.44mmol, in 40mL glacial acetic acid) was added then bromine (0.28mL, 5.48mmol, in 6mL glacial acetic acid) was added dropwise at 0 °C. The mixture was stirred at 0-5 °C for 1h. The solvents were removed. Water (50mL) and dichloromethane (100mL) were added and the organic layer was dried over $NaSO_4$. The solvents were removed, and the residue was purified by column chromatography with only hexane as eluent. The product was obtained as an oily liquid. Yield: 1.0g (57%).

Synthesis of 10-propyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-10H-phenothiazine (PTZ–Bpin)

A mixture of 3-bromo-10-propyl-10H-phenothiazine (1.5g, 4.7mmol), Bis(pinacolato)diboron (1.54g, 6.1mmol), KOAc (2.3g, 23.4mmol) and $Pd(dppf)Cl_2$ (73mg, 0.1mmol) was dissolved in 40 mL 1,4-dioxane and purged with argon for 15 minutes and refluxed the reaction mixture for overnight. After completion of reaction solvents were dried and solid residue was worked up with

dichloromethane/water. The organic layer was separated and dried over anhydrous sodium sulfate. The product was purified using column chromatography with hexane/dichloromethane (4/1 v/v). The product was obtained as fade white solid. Yield: 1.1g (64 %).



Scheme S1. Synthetic route for intermediates**:** (a) Propyl iodide, NaOH, DMSO, RT, 12 h. (b) Bromine, $CHCl_3$, AcOH, 0 °C to RT, 2 h. (c) Bis(pinacolato)diboron, KOAc, $Pd(dppf)Cl_2$, 1,4-dioxane, 80 °C, 12 h. (d-i) n-BuLi, THF, -5 °C to RT, overnight. (d-ii) p-TSA, Toluene, 90 °C, 12 h. (e) Bromine, DCM, AcOH, 0 °C to RT, 8 h.

Synthesis of (2-(4-bromophenyl)ethene-1,1,2-triyl)tribenzene (TPE–1Br)

n-BuLi (5.8mL) was added dropwise to a solution of diphenylmethane (2.0 g, 11.8 mmol) in 30 mL THF and allowed to react for 30 minutes to produce an orange-red diphenyl lithium solution and cooled it to -5 °C and then 4-bromobenzophenone (2.48 g, 9.5 mmol) was added. The reaction mixture was stirred at room temperature for overnight, and then quenched with saturated NH_4Cl solution and extracted with dichloromethane; the organic phase was dried with anhydrous Na_2SO_4 and the desiccant was removed by suction filtration. The solvent was evaporated under reduced

pressure to give the solid. Then the solid was dissolved in 25 mL toluene, and a catalytic amount of p-toluenesulfonic acid was added and allowed to reflux for 12 hours. The p-toluenesulfonic acid and the generated water were separated by an oil–water separator. The crude product was recrystallized from dichloromethane and methanol to give a white powder (3.0g). Yield: 61%.

Synthesis of 1,1,2,2-tetrakis(4-bromophenyl)ethene (TPE–4Br)

Bromine (4.0 mL, 80.0 mmol) was added to a solution of tetraphenylethylene (3.32 g, 10.0 mmol) in 10mL glacial acetic acid and dichloromethane (20 mL) at 0 °C. The resulting mixture was then stirred at room temperature for 8 h. After completion of the reaction, the reaction mixture was poured into 100 mL ice water and extracted with dichloromethane. The organic phase was dried over sodium sulphate, and the solvents were removed under reduced pressure. The crude product was purified by recrystallization with methanol and obtained a white solid (6.15 g, 95%).

Solvatochromism

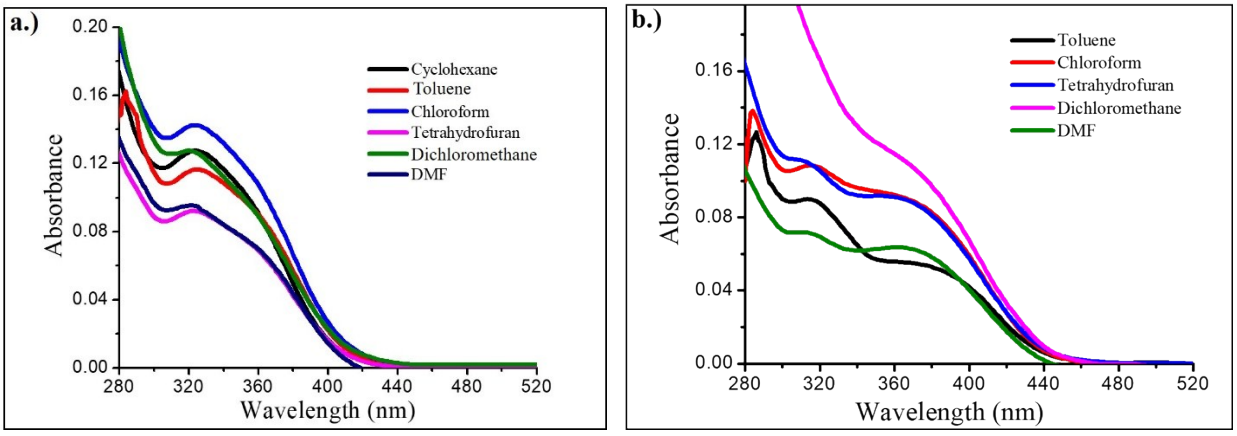


Fig. S1 Absorption spectra of compound **PTZTPE-1** (a) and **PTZTPE-4** (b) in different polarity solvents.

Table. S1 Photophysical properties of compounds **PTZTPE-1** and **PTZTPE-4** ([a] absorption and emission maxima values recorded in different polarity solvents, [b] the fluorescence quantum yields were measured using quinine sulphate as a standard in 0.5 M H_2SO_4 solution.)

Compounds	Solvent	λ_{ab}(nm)[a]	λ_{em}(nm)[a]	Stokes shift (cm^{-1})	Φ_f[b]
PTZTPE-1	Cyclohexane	324	459	9078	0.024
	Toluene	325	489	10319	0.026
	Chloroform	324	521	11670	0.006
	Tetrahydrofura	323	539	12407	0.156
	n	320	552	13134	0.155
	DCM	323	631	15112	0.019
	DMF				
PTZTPE-4	Toluene	362	564	9894	0.225
	Chloroform	358	564	10076	0.124
	Tetrahydrofura	355	574	10747	0.280
	n	355	579	10898	0.133
	DCM	362	684	12765	0.126
	DMF				

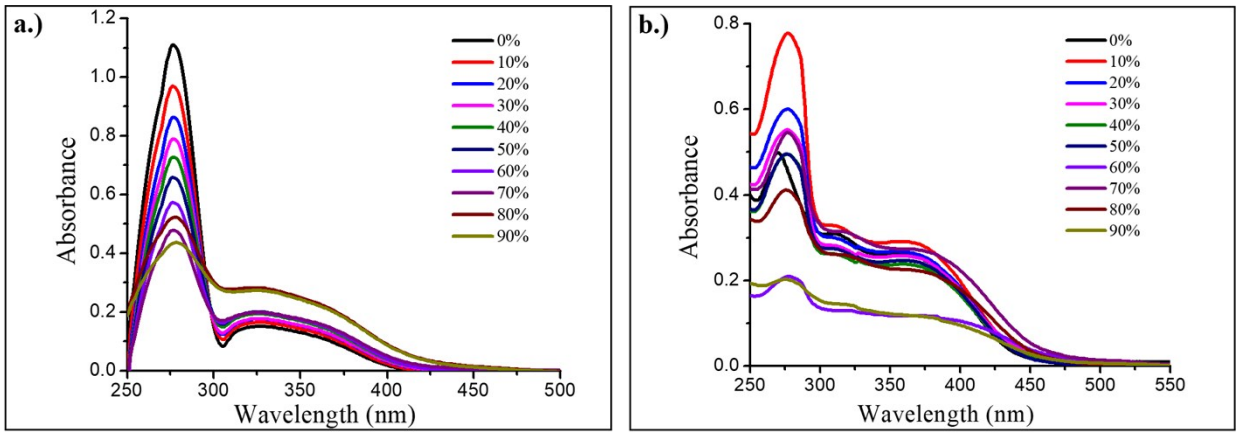
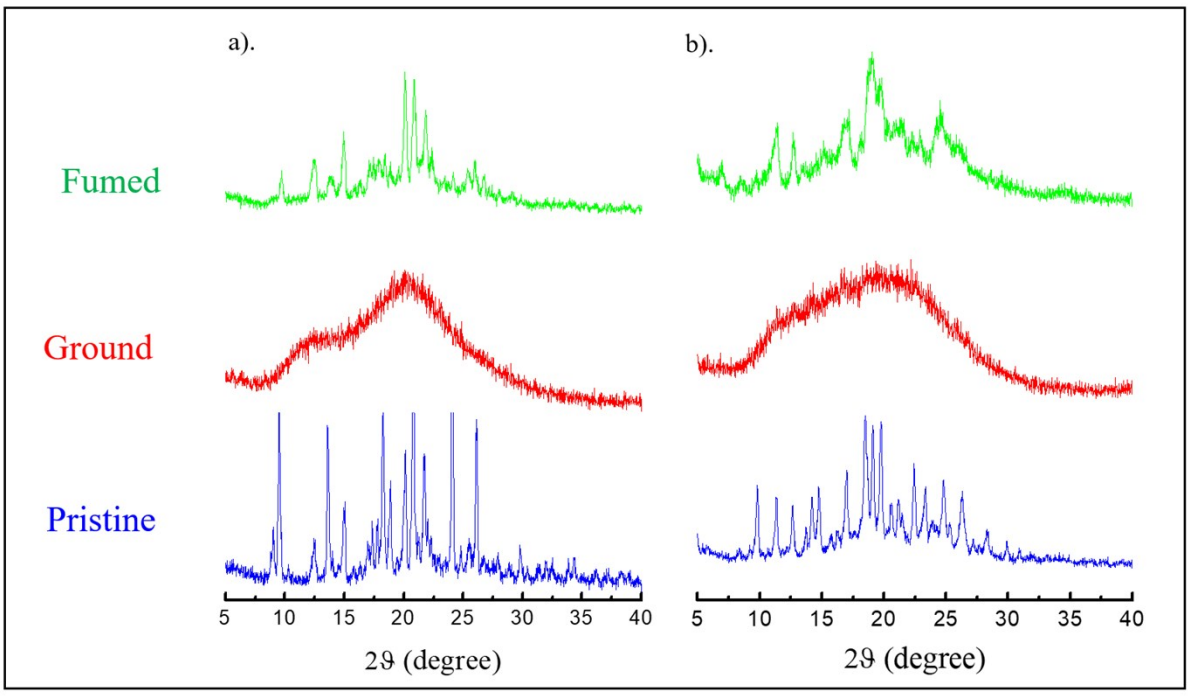


Fig. S2 Absorption spectra of compounds **PTZTPE-1** (a) and **PTZTPE-4** (b) in Water-THF mixture (0 % to 90 %).

(i)



(ii)

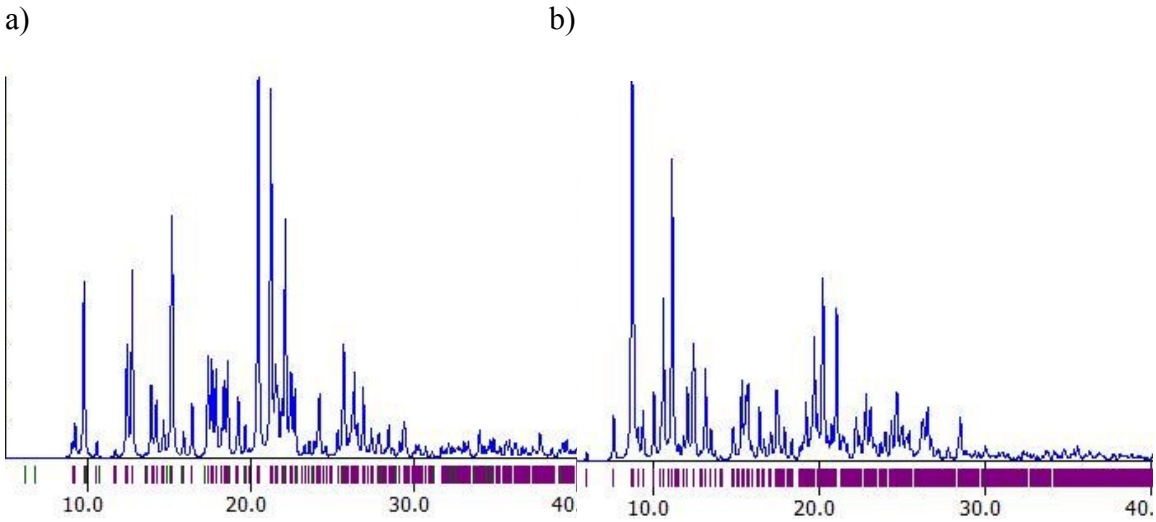


Fig. S3-(i) PXRD patterns of compound **PTZTPE-1** (a) and **PTZTPE-4** (b) in fumed, ground and pristine forms (ii) Simulated PXRD pattern for **PTZTPE-1** (a) and **PTZTPE-4** (b) derived from SC-XRD.

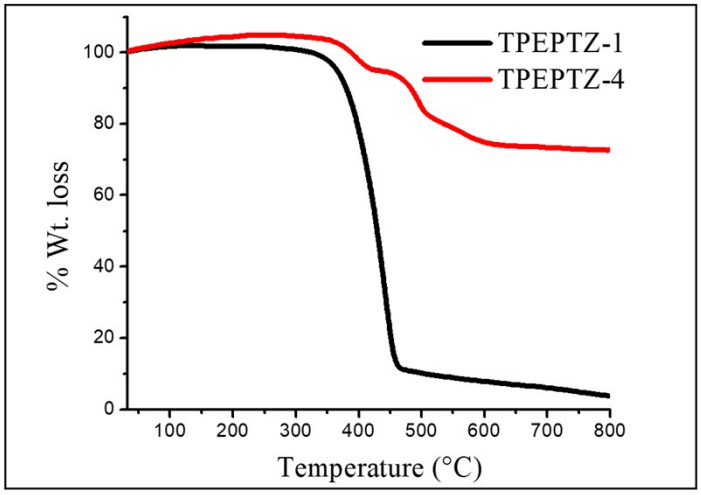


Fig. S4. TGA curve of compounds **PTZTPE-1** and **PTZTPE-4.**

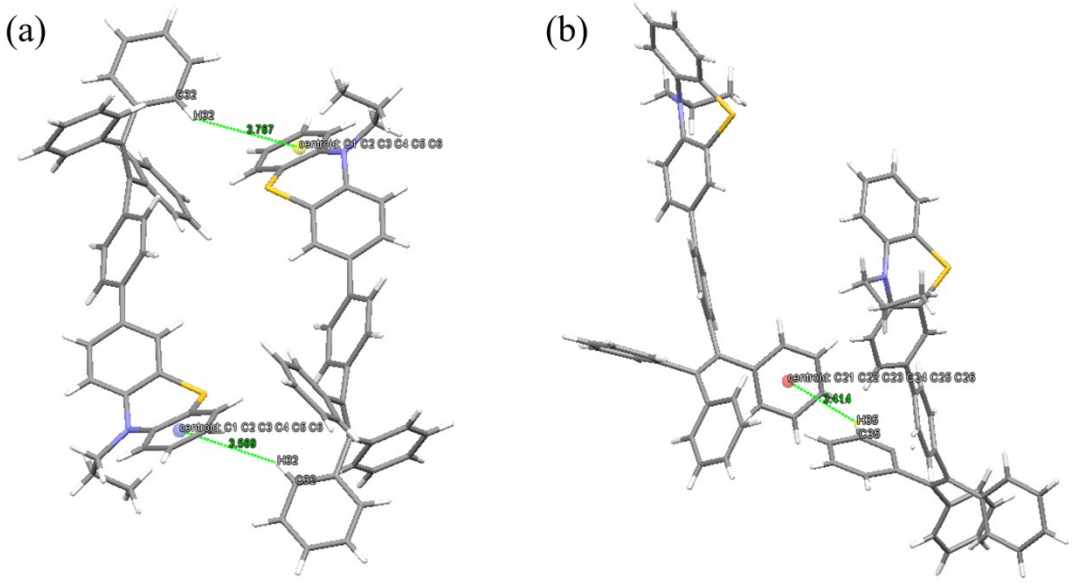


Fig. S5 Packing diagram of **PTZTPE-1** showing intermolecular interactions: (a) C(32)–H(32)…π (yellow centroid-C1–C2–C3–C4–C5–C6, 3.767 Å), C(32)–H(32)…π (blue centroid-C1–C2–C3–

C4–C5–C6, 3.569 Å) and (b) C(35)–H(35)…π (red centroid-C21–C22–C23–C24–C25–C26, 3.414 Å).

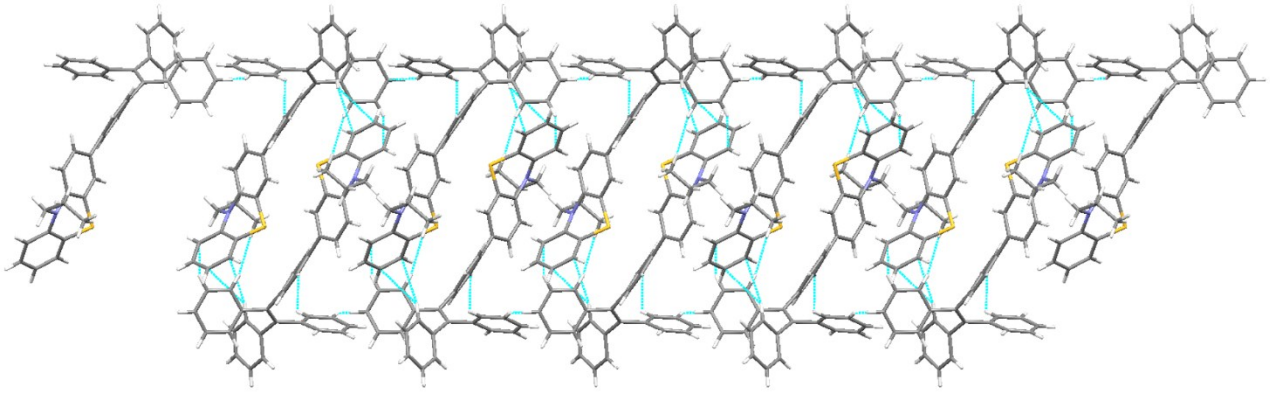


Fig. S6. Packing diagram of **PTZTPE-1** in expanded form along b axis.

Crystallographic data

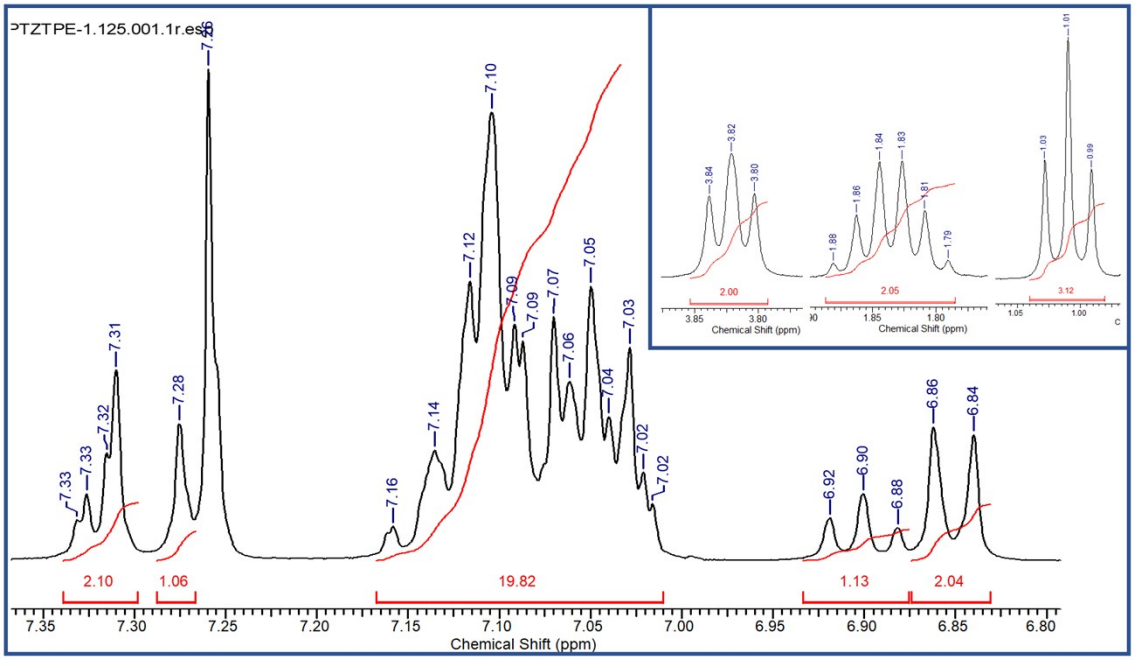
The crystal and refinement data are summarized in Table S2. The CCDC number 1917697 contains the supplementary crystallographic data for **PTZTPE-1**. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223- 336-033; or deposit@ccdc.cam.ac.uk).

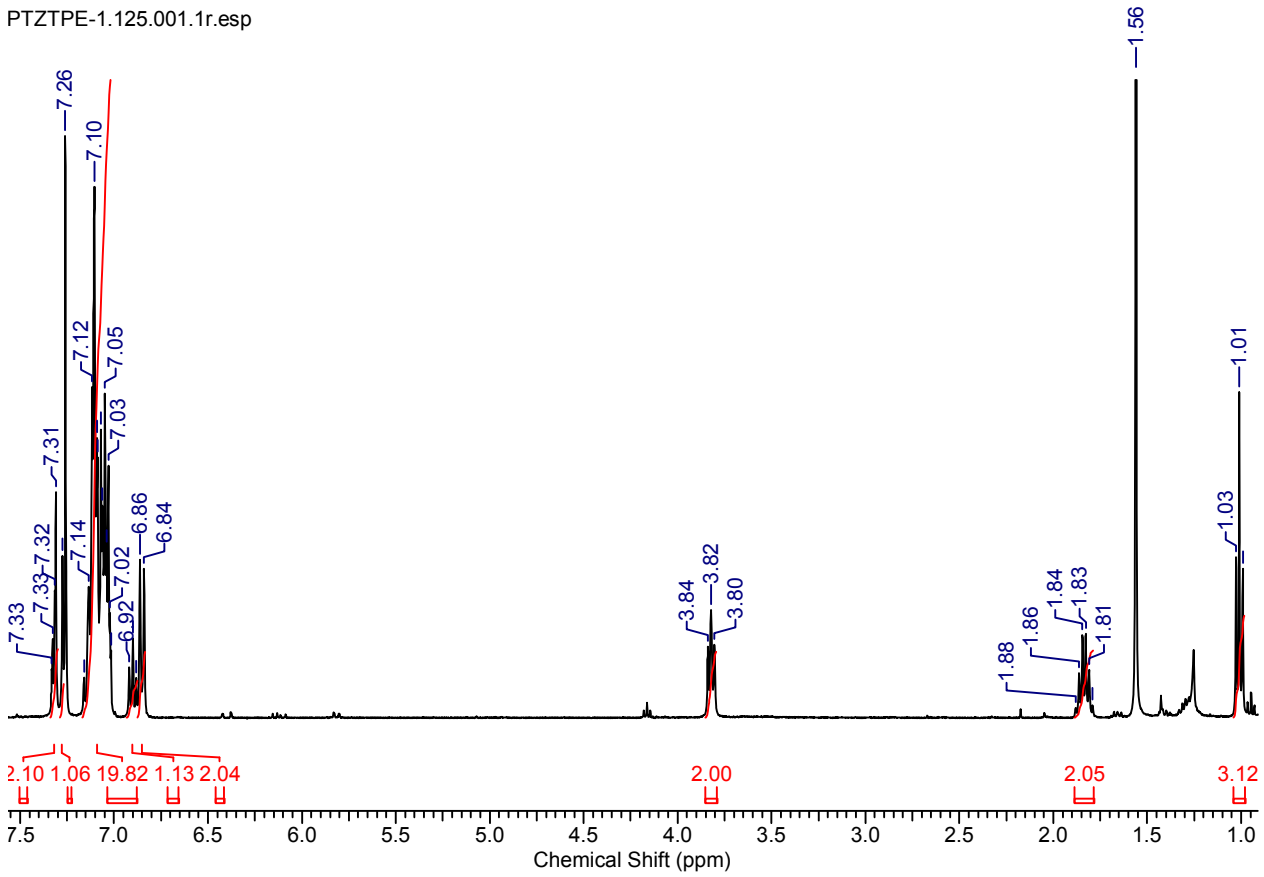
Table S2. Crystal data and structure refinement for **PTZTPE-1**.

Identification code	**PTZTPE-1**
Empirical formula	$C_{41}H_{33}NS$
Formula weight	571.74
Temperature	140(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P* 21c
a/(Å)	19.1422(13)
b/(Å)	8.1961(5)

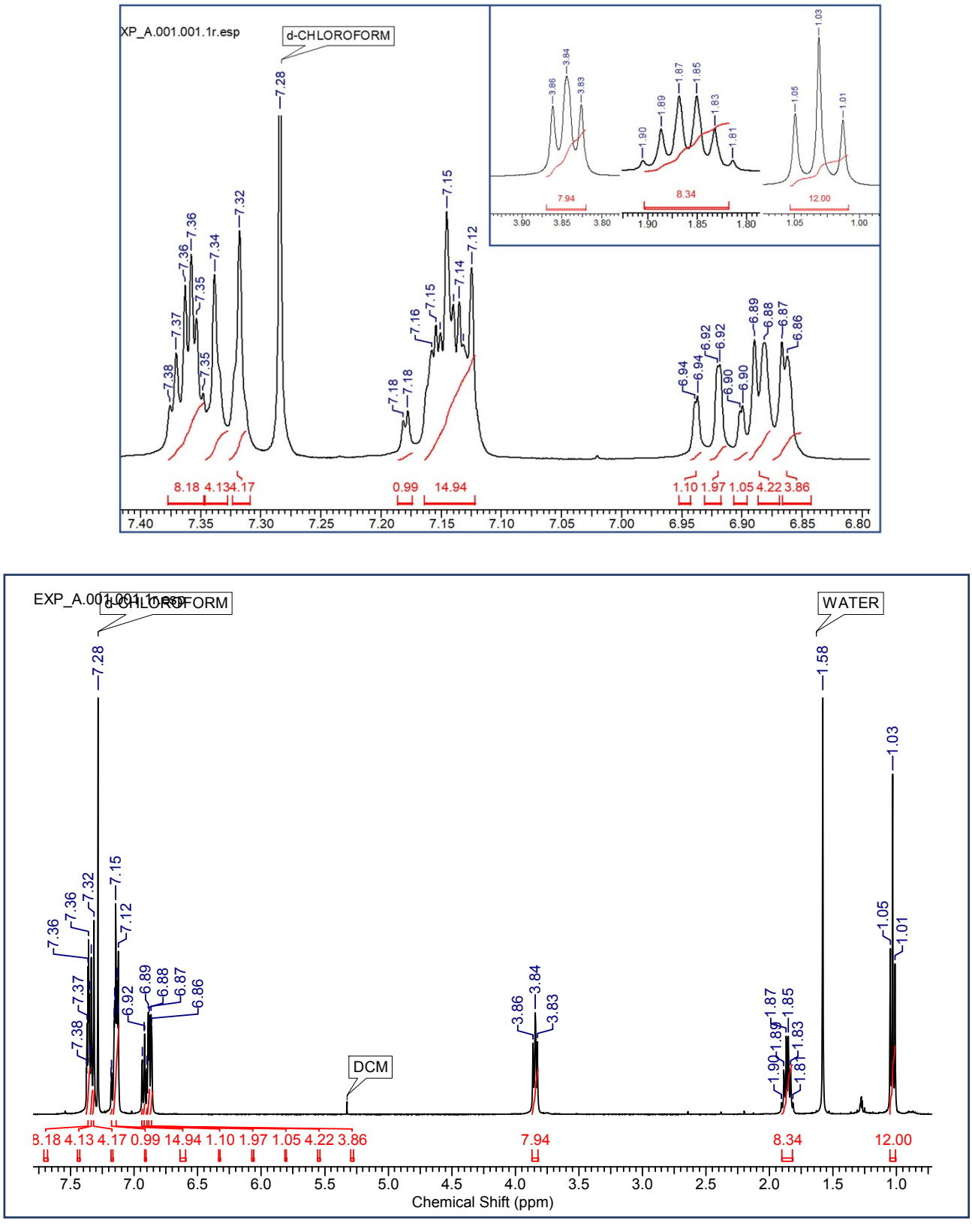
c/(Å)	19.5225(14)
Alpha/(°)	90
Beta/(°)	95.423(2)
Gamma/(°)	90
Volume	3049.2(4)
Z, calculated density	4, 1.245 mg/m^{-3}
Absorption coefficient	0.137 mm^{-1}
F(000)	1208
Crystal size	0.330 x 0.260 x 0.210 mm
Θ range for data collection/(º)	2.261 to 30.587
Reflections collected / unique	51404 / 9320 [R(int) = 0.0800]
Completeness to theta	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints /parameters	9320 / 0 / 388
Goodness-of-fit on F2	1.735
Final R indices [I>2sigma(I)]	R1 = 0.0988, wR2 = 0.2679
R indices (all data)	R1 = 0.1548, wR2 = 0.2889
Extinction coefficient	n/a
Largest diff. peak and hole ($e.Å^{-3}$)	0.893 and -0.385 $e.A^{-3}$

^{1}H-NMR spectrum of **PTZTPE-1**

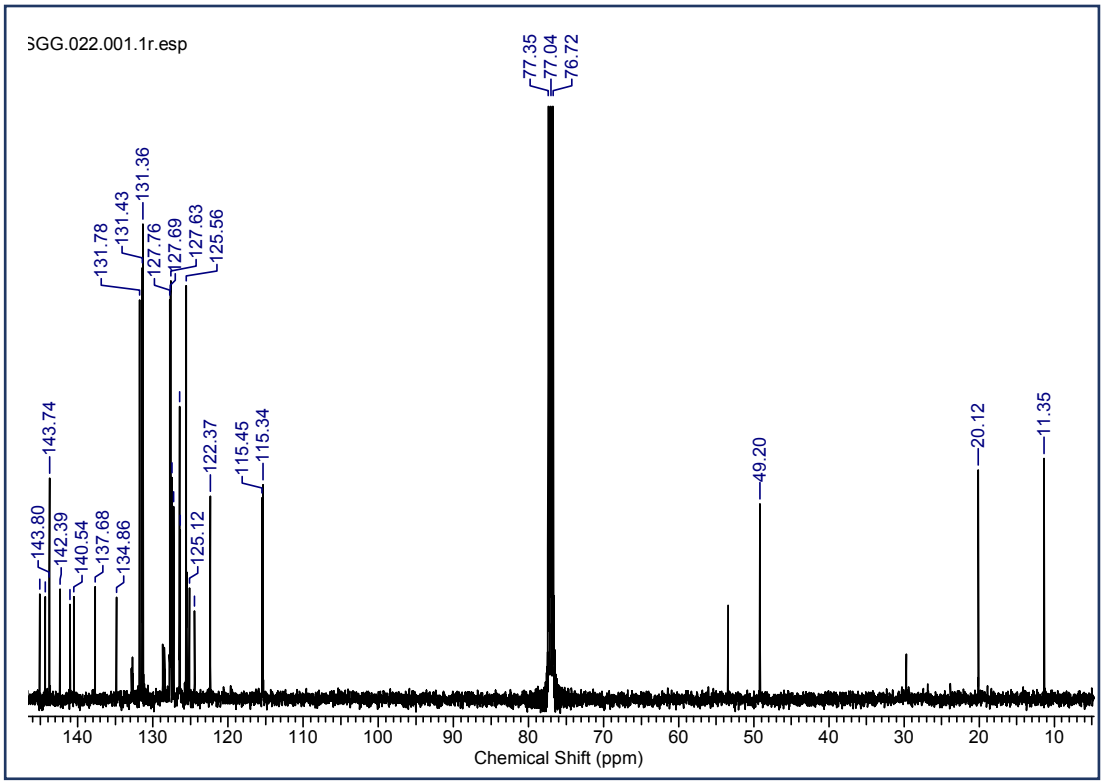




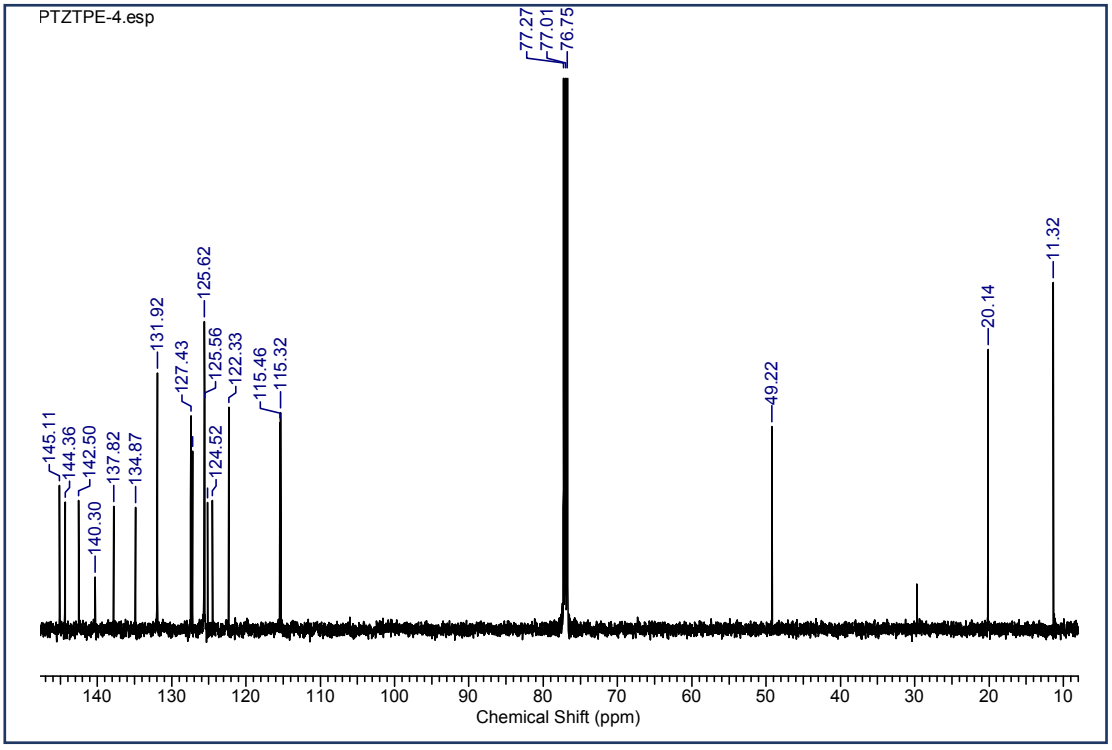
^{1}H-NMR of **PTZTPE-4**



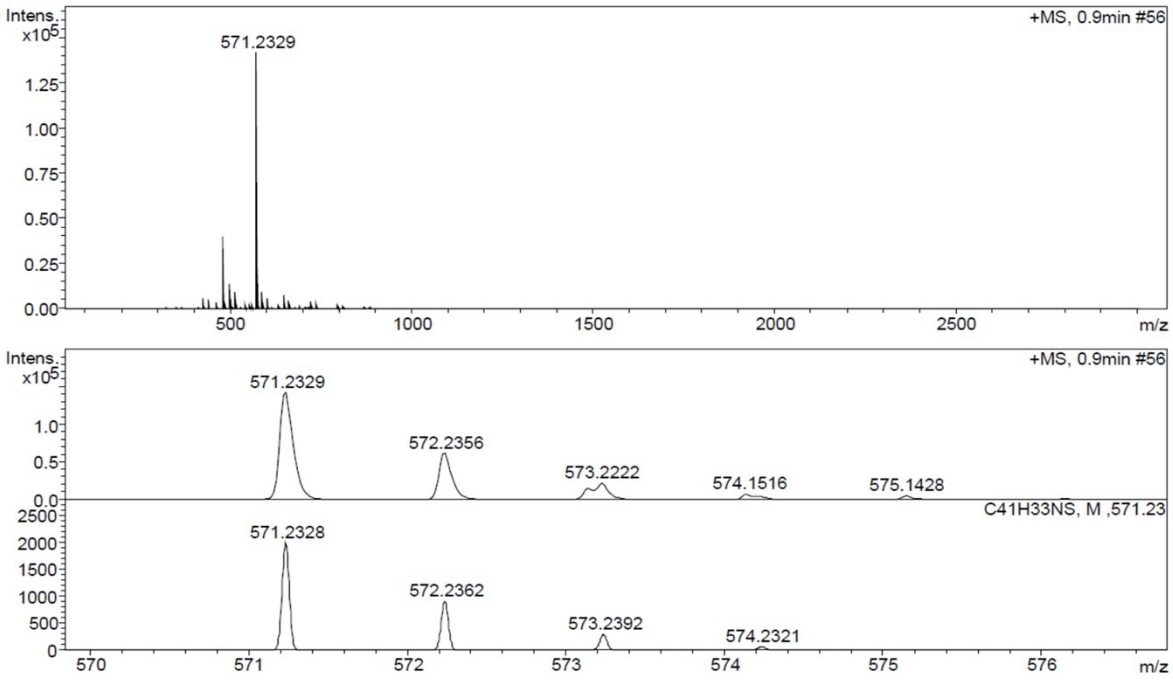
^{13}C NMR spectrum of **PTZTPE-1**



^{13}C NMR spectrum of **PTZTPE-4**



HRMS of **PTZTPE-1**



HRMS of **PTZTPE-4**

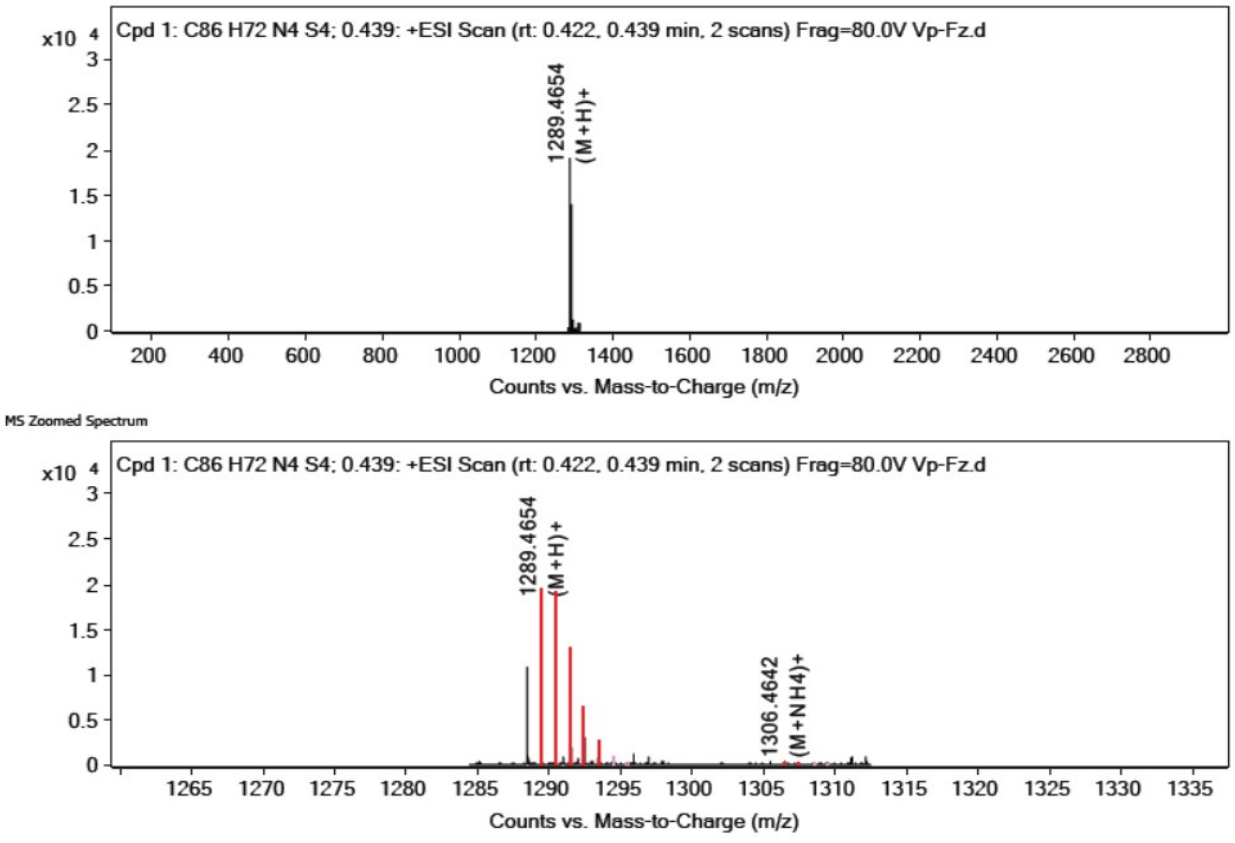


Table S3 Calculated major electronic transitions for **PTZTPE-1** and **PTZTPE-4** in the gas phase.

Compounds	Wavelength (nm)	Composition	Assignment	f^a
PTZTPE-1	377	HOMO→LUMO (0.70)	ICT	0.45
PTZTPE-4	349	HOMO→LUMO (0.70)	ICT	0.71

(Data obtained from TDDFT calculations carried out using the Gaussian 09W program performed at the B3LYP/6-31G level)

Table S4. Theoretical and electrochemical data of **PTZTPE-1** and **PTZTPE-4.**

Compounds	$E_{HOMO}{}^a$ (eV)	$E_{LUMO}{}^a$ (eV)	$E_g{}^a$ (eV)	$E_{oxid}{}^b$
PTZTPE-1	-5.22	-1.61	3.61	-0.55
PTZTPE-4	-4.80	-1.46	3.34	-0.55

(**[a]** Theoretical data obtained from DFT calculations performed using the Gaussian 09W program at B3LYP/6-31G(dp) level. **[b]** Electrochemical data obtained from CV analysis using 0.1M $TBAF_6$ as supporting electrolyte in dry DCM solvent at a scan rate of 100 mV s^{-1})

DFT calculations:

Calculation method: B3LYP/6-31G(d,p) with Gaussian 09.

PTZTPE-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.525784	0.987262	-1.403669
2	6	0	7.177348	2.035419	-2.056565
3	6	0	8.275914	2.662664	-1.463626
4	6	0	8.687877	2.260363	-0.192735
5	6	0	8.015246	1.237404	0.480848
6	6	0	6.939152	0.565665	-0.123158
7	1	0	6.827529	2.347793	-3.036065
8	1	0	9.525273	2.753341	0.292276
9	1	0	8.328645	0.971202	1.483879
10	6	0	2.801988	-0.154641	-0.848477
11	6	0	4.192803	-0.186852	-0.761614
12	6	0	4.837540	-0.495727	0.451850
13	6	0	4.031753	-0.777582	1.566103
14	6	0	2.640988	-0.779097	1.464261
15	1	0	2.343708	0.132254	-1.789869

16	1	0	4.487409	-1.012750	2.521146
17	1	0	2.052741	-1.039733	2.338709
18	7	0	6.252944	-0.501650	0.508685
19	16	0	5.193247	0.115251	-2.206656
20	1	0	8.791216	3.463440	-1.984636
21	6	0	6.924581	-1.266948	1.562714
22	1	0	6.664953	-0.896121	2.567861
23	1	0	7.996886	-1.103934	1.440444
24	6	0	6.664918	-2.777782	1.466265
25	1	0	5.591308	-2.985259	1.516729
26	1	0	7.002029	-3.120600	0.481048
27	6	0	7.391822	-3.548357	2.574364
28	1	0	7.050996	-3.237147	3.569159
29	1	0	8.475884	-3.389256	2.530061
30	1	0	7.211651	-4.624261	2.485460
31	6	0	1.993590	-0.468805	0.257785
32	6	0	0.513612	-0.459509	0.151558
33	6	0	-0.139141	-0.921383	-1.005790
34	6	0	-0.289735	0.006470	1.207631
35	6	0	-1.528869	-0.916687	-1.101029
36	1	0	0.446746	-1.317736	-1.830078
37	6	0	-1.678746	0.022736	1.106585
38	1	0	0.178766	0.384641	2.111591

39	6	0	-2.330605	-0.427886	-0.054250
40	1	0	-2.001596	-1.301037	-2.000254
41	1	0	-2.268819	0.397806	1.936632
42	6	0	-3.821273	-0.444406	-0.157909
43	6	0	-4.594292	0.639156	0.155834
44	6	0	-4.401849	-1.739709	-0.631249
45	6	0	-6.079626	0.553142	0.310521
46	6	0	-4.020319	2.003942	0.369341
47	6	0	-3.985979	-2.958591	-0.065243
48	6	0	-5.331610	-1.781210	-1.684920
49	6	0	-6.920164	1.489186	-0.319152
50	6	0	-6.672538	-0.424957	1.128105
51	6	0	-4.393083	2.770564	1.488486
52	6	0	-3.140355	2.578943	-0.564379
53	6	0	-4.506659	-4.173467	-0.513119
54	1	0	-3.252393	-2.950190	0.735792
55	6	0	-5.844107	-2.996182	-2.142526
56	1	0	-5.651709	-0.852991	-2.147418
57	6	0	-8.305886	1.428163	-0.165192
58	1	0	-6.481540	2.266664	-0.938053
59	6	0	-8.057359	-0.479401	1.293719
60	1	0	-6.040579	-1.144767	1.638378
61	6	0	-3.876879	4.052225	1.685238

62	1	0	-5.088736	2.354298	2.211497
63	6	0	-2.633132	3.865427	-0.375729
64	1	0	-2.854734	2.011042	-1.444097
65	6	0	-5.439138	-4.197802	-1.554624
66	1	0	-4.180321	-5.101396	-0.051715
67	1	0	-6.558250	-3.003335	-2.961221
68	6	0	-8.881470	0.442568	0.642461
69	1	0	-8.935778	2.153854	-0.672203
70	1	0	-8.491750	-1.241764	1.934395
71	6	0	-2.993633	4.605947	0.753544
72	1	0	-4.168884	4.620515	2.564020
73	1	0	-1.957780	4.289787	-1.113355
74	1	0	-5.839882	-5.143214	-1.908857
75	1	0	-9.959426	0.398670	0.768755
76	1	0	-2.596937	5.606128	0.902157

Rotational constants (GHZ): 0.1516757 0.0284419 0.0261809

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TD-DFT calculations:

PTZTPE-1

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2856 eV 377.36 nm f=0.4547 <S**2>=0.000

151 ->152 0.69149

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2035.11901444

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6410 eV 340.52 nm f=0.2401 <S**2>=0.000

150 ->152 0.68779

Excited State 3: Singlet-A 3.8020 eV 326.10 nm f=0.0478 <S**2>=0.000

150 ->152 0.11498

151 ->152 0.11218

151 ->153 0.58224

151 ->154 -0.19390

151 ->155 -0.16746

151 ->156 0.18228

Excited State 4: Singlet-A 4.0070 eV 309.42 nm f=0.1091 <S**2>=0.000

149 ->152 -0.17637

151 ->153 0.28552

151 ->154 0.46955

151 ->155 0.33324

Excited State 5: Singlet-A 4.1362 eV 299.75 nm f=0.1499 <S**2>=0.000

150 ->153 0.21768

151 ->153 -0.13143

151 ->154 0.14512

151 ->155 0.10377

151 ->156 0.58919

151 ->157 0.10914

Excited State 6: Singlet-A 4.2201 eV 293.79 nm f=0.0110 <S**2>=0.000

150 ->153 0.40476

150 ->154 -0.15377

150 ->155 0.10329

151 ->154 0.22691

151 ->155 -0.34973

151 ->156 -0.10717

151 ->157 -0.20454

151 ->158 -0.10373

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

****

DFT calculations:

Calculation method: B3LYP/6-31G(d,p) with Gaussian 09.

PTZTPE-4

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

1	6	0	3.565314	-3.238148	0.348635
2	6	0	2.571169	-3.565612	-0.589641
3	6	0	3.368630	-2.083205	1.125524
4	6	0	1.438511	-2.773884	-0.745460
5	1	0	2.672261	-4.469198	-1.183347
6	6	0	2.239764	-1.287552	0.964622
7	1	0	4.121495	-1.792269	1.851911
8	6	0	1.252923	-1.606421	0.016103
9	1	0	0.679383	-3.064335	-1.465244
10	1	0	2.120177	-0.400108	1.576907
11	6	0	0.020631	-0.779369	-0.142181
12	6	0	0.048351	0.586661	-0.225519
13	6	0	-1.252610	-1.557562	-0.204272
14	6	0	-1.182419	1.422641	-0.098230
15	6	0	1.306812	1.358055	-0.446673
16	6	0	-1.522601	-2.575825	0.726738
17	6	0	-2.196110	-1.340466	-1.222168
18	6	0	-1.444220	2.463350	-1.006655
19	6	0	-2.087133	1.242431	0.961399
20	6	0	1.592613	2.502539	0.318409
21	6	0	2.219386	1.007614	-1.456308
22	6	0	-2.697261	-3.317828	0.663347
23	1	0	-0.798168	-2.787640	1.507383

24	6	0	-3.365608	-2.089851	-1.292217
25	1	0	-2.010032	-0.567970	-1.960905
26	6	0	-2.574317	3.264068	-0.880360
27	1	0	-0.747578	2.646867	-1.819064
28	6	0	-3.211483	2.050027	1.094007
29	1	0	-1.906382	0.453693	1.684025
30	6	0	2.752747	3.239837	0.108285
31	1	0	0.901816	2.805331	1.099380
32	6	0	3.371399	1.754467	-1.677198
33	1	0	2.012200	0.146293	-2.082745
34	6	0	-3.647289	-3.091576	-0.347716
35	1	0	-2.868392	-4.105962	1.390601
36	1	0	-4.083957	-1.879293	-2.078891
37	6	0	-3.485325	3.076089	0.173502
38	1	0	-2.738280	4.068371	-1.591350
39	1	0	-3.901077	1.868061	1.912849
40	6	0	3.670172	2.884065	-0.895541
41	1	0	2.962943	4.091384	0.748429
42	1	0	4.036237	1.476334	-2.489480
43	6	0	4.902938	3.673635	-1.125083
44	6	0	4.912780	5.068772	-0.958614
45	6	0	6.106050	3.060131	-1.505330
46	6	0	6.061320	5.817817	-1.195753

47	1	0	4.000514	5.586292	-0.679299
48	6	0	7.267883	3.800428	-1.708548
49	1	0	6.148541	1.979962	-1.603787
50	6	0	7.267869	5.196833	-1.572583
51	16	0	6.007311	7.599079	-1.110886
52	1	0	8.183997	3.281651	-1.966745
53	7	0	8.422610	5.984614	-1.787890
54	6	0	7.639364	7.862314	-0.441620
55	6	0	8.693766	7.033859	-0.874245
56	6	0	9.504569	5.459257	-2.623749
57	6	0	7.872831	8.905181	0.454628
58	6	0	9.979268	7.278490	-0.366877
59	1	0	9.951690	4.548760	-2.193201
60	1	0	10.293036	6.213887	-2.634213
61	6	0	9.072841	5.207537	-4.075406
62	6	0	9.164884	9.166726	0.912026
63	1	0	7.037985	9.518118	0.780558
64	6	0	10.213508	8.347489	0.499087
65	1	0	10.802763	6.628489	-0.639832
66	1	0	8.245624	4.491699	-4.106743
67	1	0	8.685078	6.147481	-4.484061
68	6	0	10.234306	4.693718	-4.931382
69	1	0	9.343527	9.993080	1.592554

70	1	0	11.221033	8.522689	0.864282
71	1	0	10.622975	3.741990	-4.551107
72	1	0	11.066390	5.406808	-4.949606
73	1	0	9.916363	4.530439	-5.965293
74	6	0	-4.687574	3.931763	0.313522
75	6	0	-5.156234	4.322115	1.579150
76	6	0	-5.400280	4.383912	-0.806850
77	6	0	-6.307477	5.092057	1.718513
78	1	0	-4.611267	4.030574	2.471225
79	6	0	-6.531060	5.186126	-0.674781
80	1	0	-5.076997	4.092641	-1.801252
81	6	0	-7.019639	5.543213	0.590836
82	16	0	-6.942615	5.473661	3.340832
83	1	0	-7.043782	5.523294	-1.568298
84	7	0	-8.179076	6.335689	0.765617
85	6	0	-7.555559	7.111839	2.992439
86	6	0	-8.141188	7.366913	1.736406
87	6	0	-9.181580	6.385119	-0.301314
88	6	0	-7.503429	8.104580	3.970763
89	6	0	-8.656402	8.649982	1.494529
90	1	0	-8.773941	6.817540	-1.229283
91	1	0	-9.968885	7.062756	0.033883
92	6	0	-9.822724	5.019323	-0.584418

93	6	0	-8.063404	9.360244	3.732559
94	1	0	-7.033734	7.882264	4.924120
95	6	0	-8.636656	9.626790	2.490913
96	1	0	-9.068089	8.894600	0.521993
97	1	0	-9.056506	4.292106	-0.870180
98	1	0	-10.267543	4.651458	0.347068
99	6	0	-10.885584	5.108663	-1.683611
100	1	0	-8.038819	10.121797	4.505412
101	1	0	-9.056082	10.606211	2.281107
102	1	0	-10.455242	5.455978	-2.629968
103	1	0	-11.688757	5.802805	-1.411088
104	1	0	-11.341403	4.131439	-1.867751
105	6	0	-4.898775	-3.882825	-0.418350
106	6	0	-5.447697	-4.263774	-1.654146
107	6	0	-5.579975	-4.280949	0.741372
108	6	0	-6.643352	-4.973056	-1.726668
109	1	0	-4.931528	-4.013314	-2.575384
110	6	0	-6.756928	-5.022639	0.675616
111	1	0	-5.193964	-3.994298	1.714548
112	6	0	-7.323268	-5.370757	-0.559733
113	16	0	-7.374160	-5.344232	-3.310731
114	1	0	-7.243450	-5.319252	1.597642
115	7	0	-8.528451	-6.105181	-0.667291

116	6	0	-8.048926	-6.944945	-2.906681
117	6	0	-8.586597	-7.151830	-1.620663
118	6	0	-9.477301	-6.091588	0.448739
119	6	0	-8.089739	-7.954081	-3.868598
120	6	0	-9.151087	-8.404353	-1.332904
121	1	0	-9.044002	-6.529791	1.362257
122	1	0	-10.311613	-6.735396	0.164703
123	6	0	-10.037066	-4.692199	0.740296
124	6	0	-8.697080	-9.177358	-3.582703
125	1	0	-7.654924	-7.769528	-4.846251
126	6	0	-9.224139	-9.396361	-2.311640
127	1	0	-9.528196	-8.613601	-0.338382
128	1	0	-9.222195	-3.998412	0.969196
129	1	0	-10.514984	-4.318881	-0.172431
130	6	0	-11.040132	-4.711271	1.897475
131	1	0	-8.744689	-9.951191	-4.342176
132	1	0	-9.679669	-10.350891	-2.065532
133	1	0	-10.574010	-5.059212	2.826463
134	1	0	-11.887444	-5.373207	1.684727
135	1	0	-11.441004	-3.710802	2.084504
136	6	0	4.771574	-4.082841	0.517607
137	6	0	5.358453	-4.266659	1.780976
138	6	0	5.371367	-4.731136	-0.572392

139	6	0	6.513447	-5.027223	1.939112
140	1	0	4.904203	-3.818939	2.658955
141	6	0	6.503779	-5.526198	-0.413902
142	1	0	4.956367	-4.603282	-1.567140
143	6	0	7.110057	-5.677685	0.842108
144	16	0	7.300308	-5.144357	3.535317
145	1	0	6.924936	-6.020287	-1.281991
146	7	0	8.274703	-6.456911	1.039455
147	6	0	7.863890	-6.832015	3.414610
148	6	0	8.322307	-7.309224	2.170626
149	6	0	9.166535	-6.714101	-0.093668
150	6	0	7.899028	-7.644240	4.547950
151	6	0	8.800804	-8.626973	2.102646
152	1	0	8.667158	-7.291763	-0.888179
153	1	0	9.978915	-7.341243	0.277840
154	6	0	9.786577	-5.434298	-0.672271
155	6	0	8.422868	-8.935419	4.474765
156	1	0	7.526215	-7.253173	5.489728
157	6	0	8.870069	-9.421310	3.247906
158	1	0	9.113673	-9.042211	1.151462
159	1	0	9.001952	-4.752227	-1.013910
160	1	0	10.317304	-4.917160	0.135009
161	6	0	10.744180	-5.741429	-1.827604

162	1	0	8.467418	-9.555140	5.364611
163	1	0	9.258907	-10.432132	3.168882
164	1	0	10.227794	-6.242538	-2.654443
165	1	0	11.564715	-6.393170	-1.506705
166	1	0	11.187175	-4.822999	-2.223824

Rotational constants (GHZ): 0.0109051 0.0074880 0.0048705

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TD-DFT calculations:

PTZTPE-4

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: Singlet-?Sym 2.9333 eV 422.67 nm f=0.7132 <S**2>=0.000

340 -> 341 0.69497

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -5132.34109292

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: Singlet-?Sym 3.1652 eV 391.71 nm f=0.0175 <S**2>=0.000

338 -> 341 0.68048

339 -> 341 -0.12496

Excited state symmetry could not be determined.

Excited State 3: Singlet-?Sym 3.1736 eV 390.67 nm f=0.3528 <S**2>=0.000

337 -> 341 -0.16309

338 -> 341 0.12911

339 -> 341 0.66273

Excited state symmetry could not be determined.

Excited State 4: Singlet-?Sym 3.2333 eV 383.46 nm f=0.0562 <S**2>=0.000

337 -> 341 0.67752

339 -> 341 0.16819

Excited state symmetry could not be determined.

Excited State 5: Singlet-?Sym 3.4985 eV 354.39 nm f=0.1449 <S**2>=0.000

336 -> 341 0.68787

Excited state symmetry could not be determined.

Excited State 6: Singlet-?Sym 3.5508 eV 349.17 nm f=0.7886 <S**2>=0.000

337 -> 343 -0.12584

338 -> 344 -0.13613

340 -> 342 0.65113

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

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