Supplementary Materials for

Stabilizing 4π Electron Pyrrolyl Cation by inducing aromaticity

The PDF file includes:

Materials and Methods
Supplementary Text
NMR spectra
Figs. S1 to S35
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References

Other Supplementary Materials for this manuscript include the following:

XYZ Coordinates

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General considerations

All the reagents were obtained from commercial sources and were used as such without any purification. Organic solvents used for reaction were purified and dried over appropriate drying agents according to the standard methods prior to use. The reactions were monitored by thin layer chromatography (TLC) using 0.2 mm Merck pre-coated silica gel 60 F254 aluminium sheets. The intermediate products were purified by column chromatography using 100-200 mesh size silica gel as stationary bed and ethyl acetate/*n*-hexane as mobile phase. Melting points (MPs) were measured using a Cole-Parmer MP-400 melting point apparatus. Proton nuclear magnetic resonance (^{1}H NMR) and carbon NMR (^{13}C NMR) spectra were recorded on JEOL ECA 600 MHz spectrometer. ^{1}H chemical shifts (δ) are given in ppm and coupling constant (*J*) values are given in hertz. The chemical shifts are referenced to NMR residual solvents ($CDCl_3$, ^{1}H δ = 7.25, ^{13}C δ = 77.0; DMSO-d_6, ^{1}H δ = 2.50, ^{13}C δ = 39.53; and CD_3OD ^{1}H δ = 3.31, ^{13}C δ = 49.03. Splitting pattern were abbreviated as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, dt = doublet of triplet, hept = heptet and m = multiplet. ^{13}C NMR was recorded at 151 MHz after fully decoupled broad band decoupling. UV-Vis data was collected using Shimadzu UV-2450 instrument. Emission spectra was collected using Cary Eclipse Fluorescence Spectrophotometer.

Table S1. The experimental and quantum chemically estimated values of ^{1}H NMR of compounds **3a-3d** using M06-2x/def2tzvpp level of theory.

	Experimental		Theoretical	
Compound	**NH proton δ (ppm)**	**Pyrrole aromatic δ (ppm)**	**NH proton δ (ppm)**	**Pyrrole aromatic δ (ppm)**
3a	10.74	5.41	10.67	5.29
3b	11.77	6.97	10.67	7.17
3c	10.8	6.41	10.47	6.93
3d	10.52	6.89	10.35	7.02

Table S2. The experimental and quantum chemically estimated values of ^{1}H NMR of compounds **4a-4d** using M06-2x/def2tzvpp level of theory.

	^{1}H NMR Pyrrolyl cation H_4 (in ppm)	
Compound	**Experimental**	**Theoretical**
4a	5.79	5.61
4b	7.39	7.43
4c	7.13	7.33
4d	7.56	7.59

The computational results obtained from the calculation have been scaled by 0.91. Although the scaling factor for this basis set (M06-2x/def2tzvpp) was not found in literature, the scaling factor 0.91 was chosen by comparing with nearest match.[1]

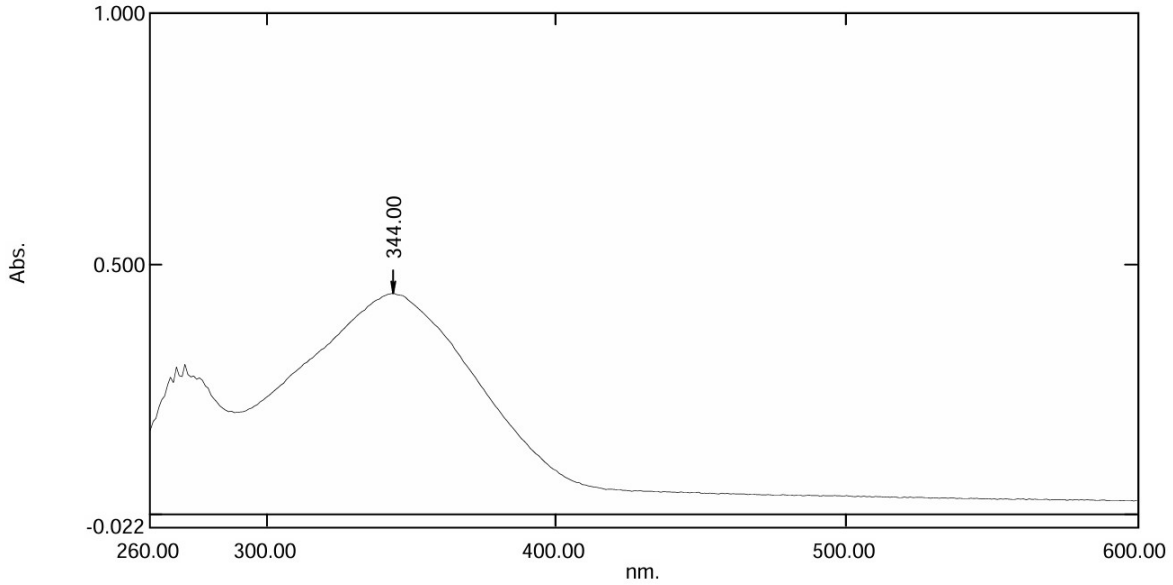


Figure S1: Experimental UV-Vis analysis of **4a**. Experimental UV-Vis was obtained from a 10^{-4} M solution of **4a** in dry acetonitrile. A broad peak at 344 nm was observed.

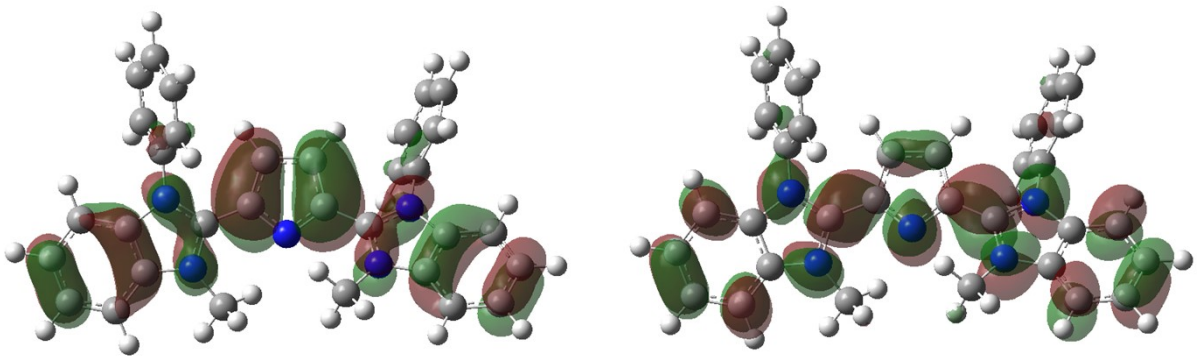


Figure S2. Electronic transitions corresponding to the calculated bands, along with their percentage contributions to the absorption.

Table S3. TD-DFT computed UV-Vis spectrum for compound **4a**.

Compound	Experimental λ_{max} (nm)	Calculated λ_{max} (nm)	Oscillator Strength (f)
4a	344	347	1.4557

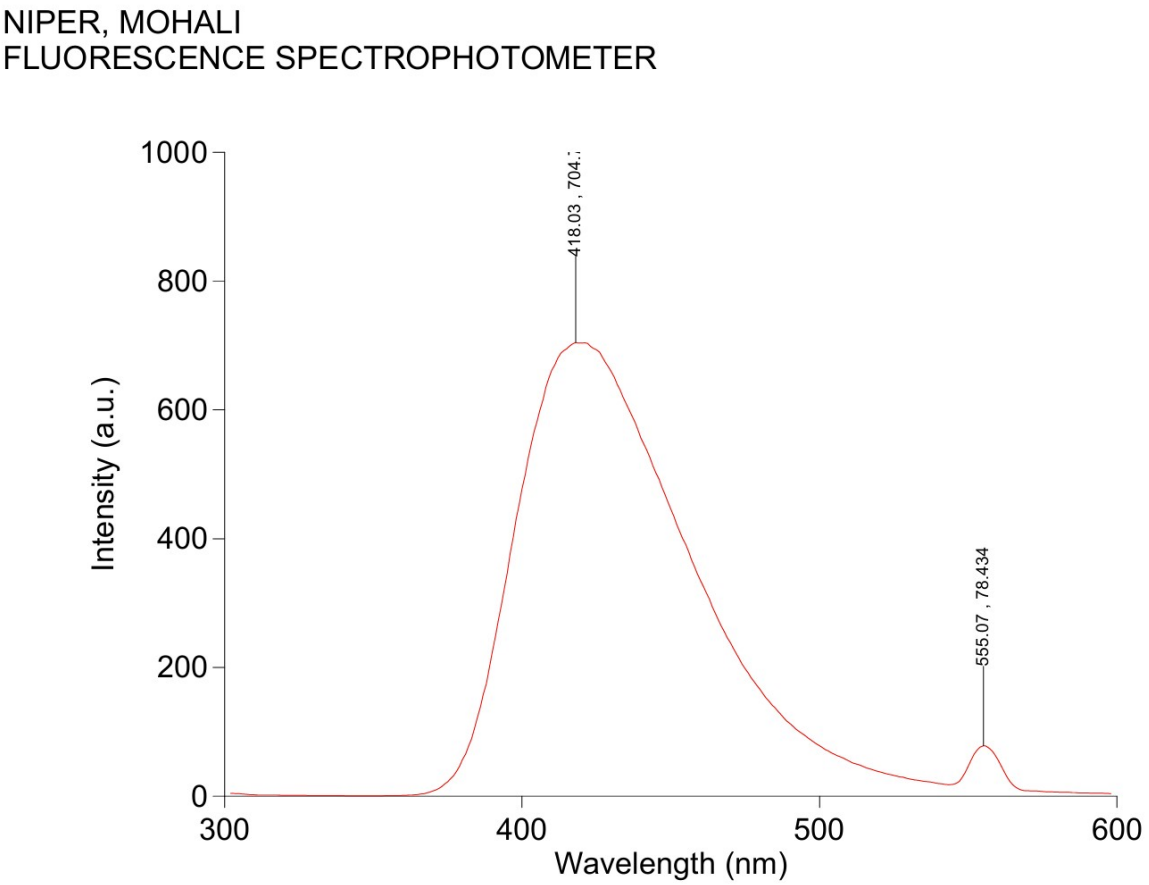


Figure S3: Experimental Emission spectrum of **4a**. Experimental Fluorescence spectrum was obtained from a 10^{-4} M solution of **4a** in dry acetonitrile. A broad peak at 418 nm was observed.

Table S4. TD-DFT computed Emission spectrum for compound **4a**.

S. No.	Experimental			opt def2tzvpp m062x n=6		
	Wavelength (nm)	Emission Intensity (a.u.)	Energy (eV)	Wavelength (nm)	Energy (eV)	f
4a	418.03	704.73	2.97	428.32	2.89	1.84

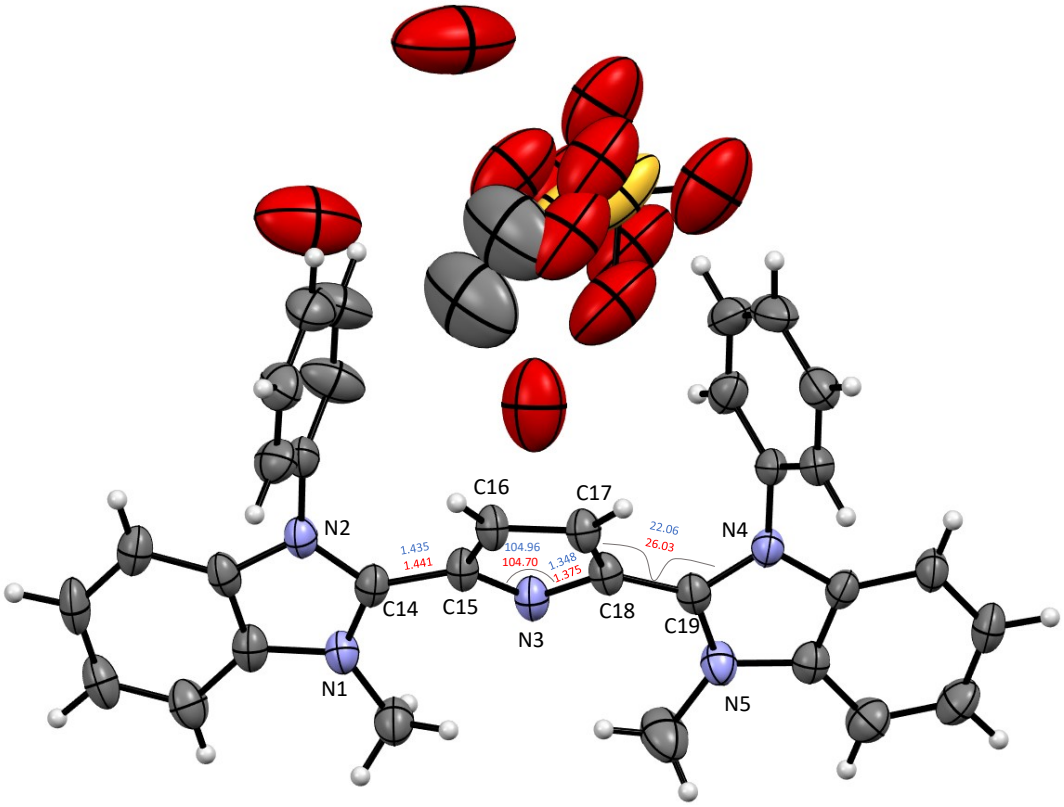


Figure S4. Comparison of the geometrical parameters of **4a** obtained using X-ray diffraction (red colour) and M06-2X/def2tzvpp (blue colour). Thermal ellipsoids are drawn at the 50% probability level.

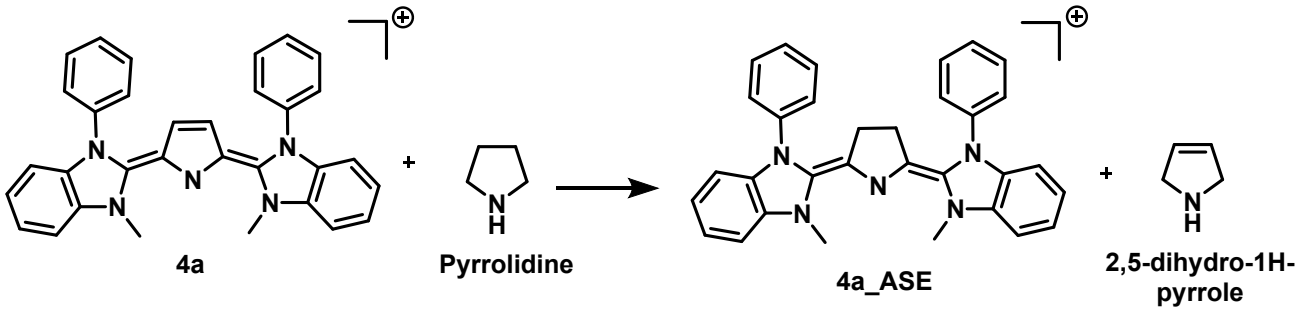


Figure S5. Equation employed to estimate the aromatic stabilization energy (ASE) of **4a**. Similar equations were used for **4b**-**4f**, and **5**.

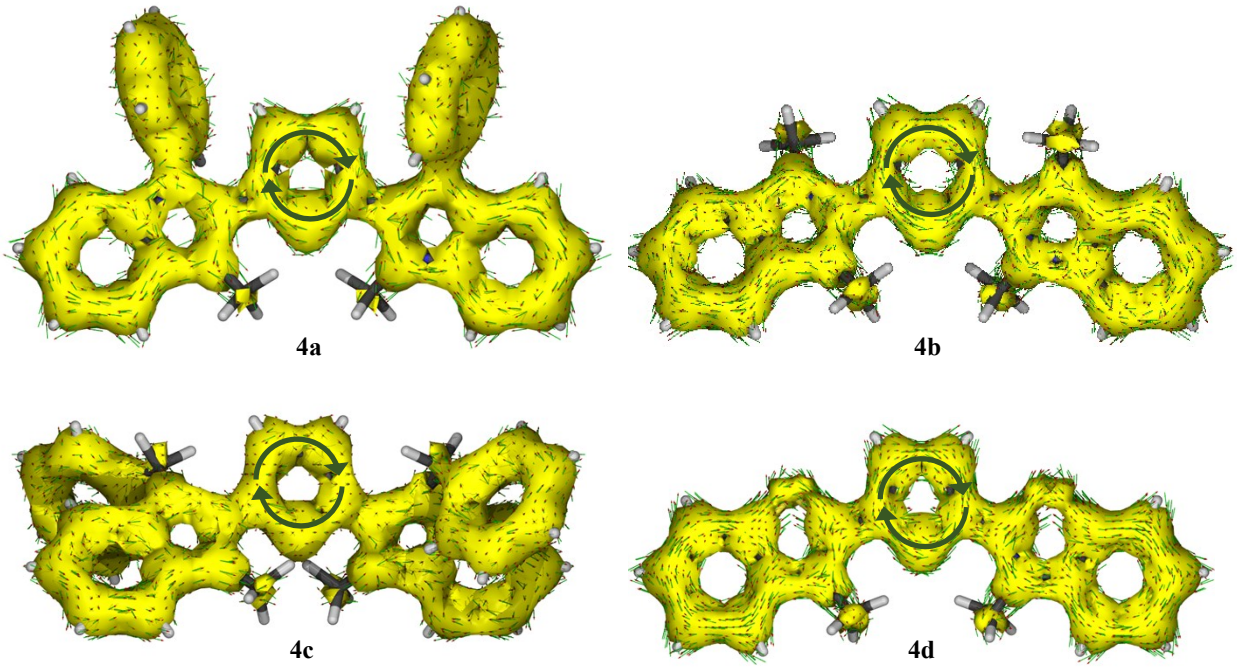


Figure S6. Contour diagrams generated for compounds (**4a-4d**) using ACID analysis. Clockwise direction of arrows indicates aromatic character in the ring.

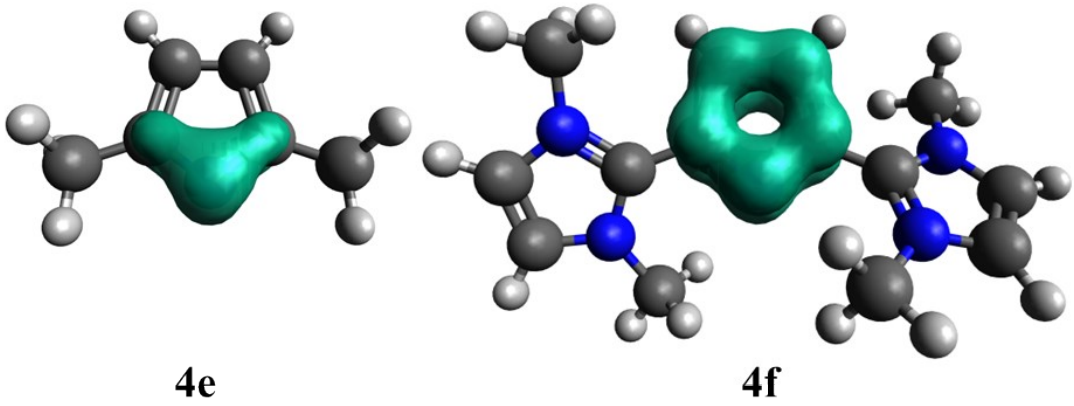


Figure S7. The EDDB contour maps (with an isosurface value of 0.015 a.u.) of **4e** and **4f**. The total number of delocalized electrons in the central ring particularly could be estimated using $EDDB_{P,}$ which is 0.858 for **4e** indicating negligible delocalization and 3.904 (Table 1 in main manuscript) for the central ring of **4f** showing significant delocalization in the central pyrrolyl cation ring.

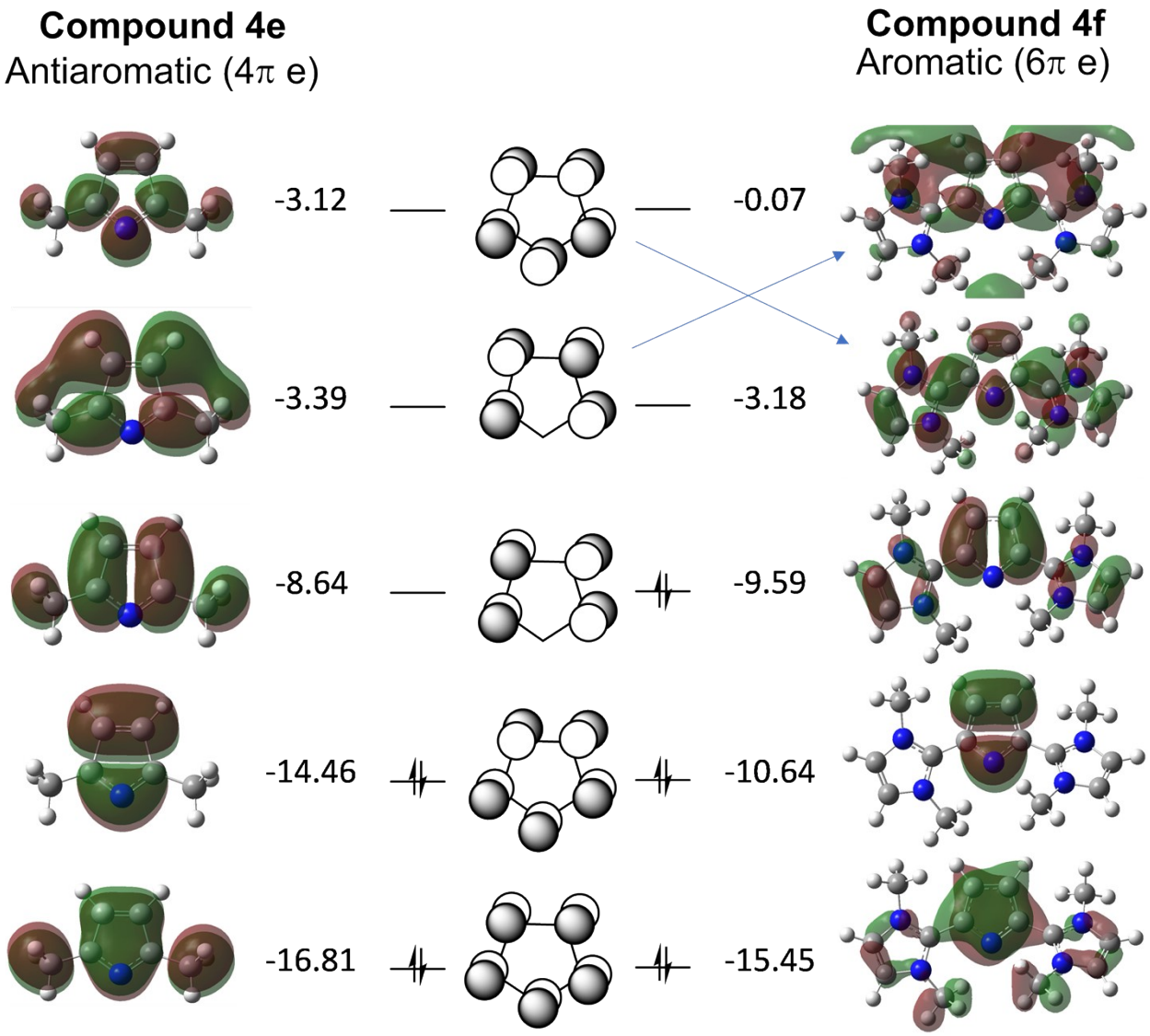


Figure S8. Frontier Molecular π Orbitals of **4e** and **4f**. The molecular orbital energies are in eV.

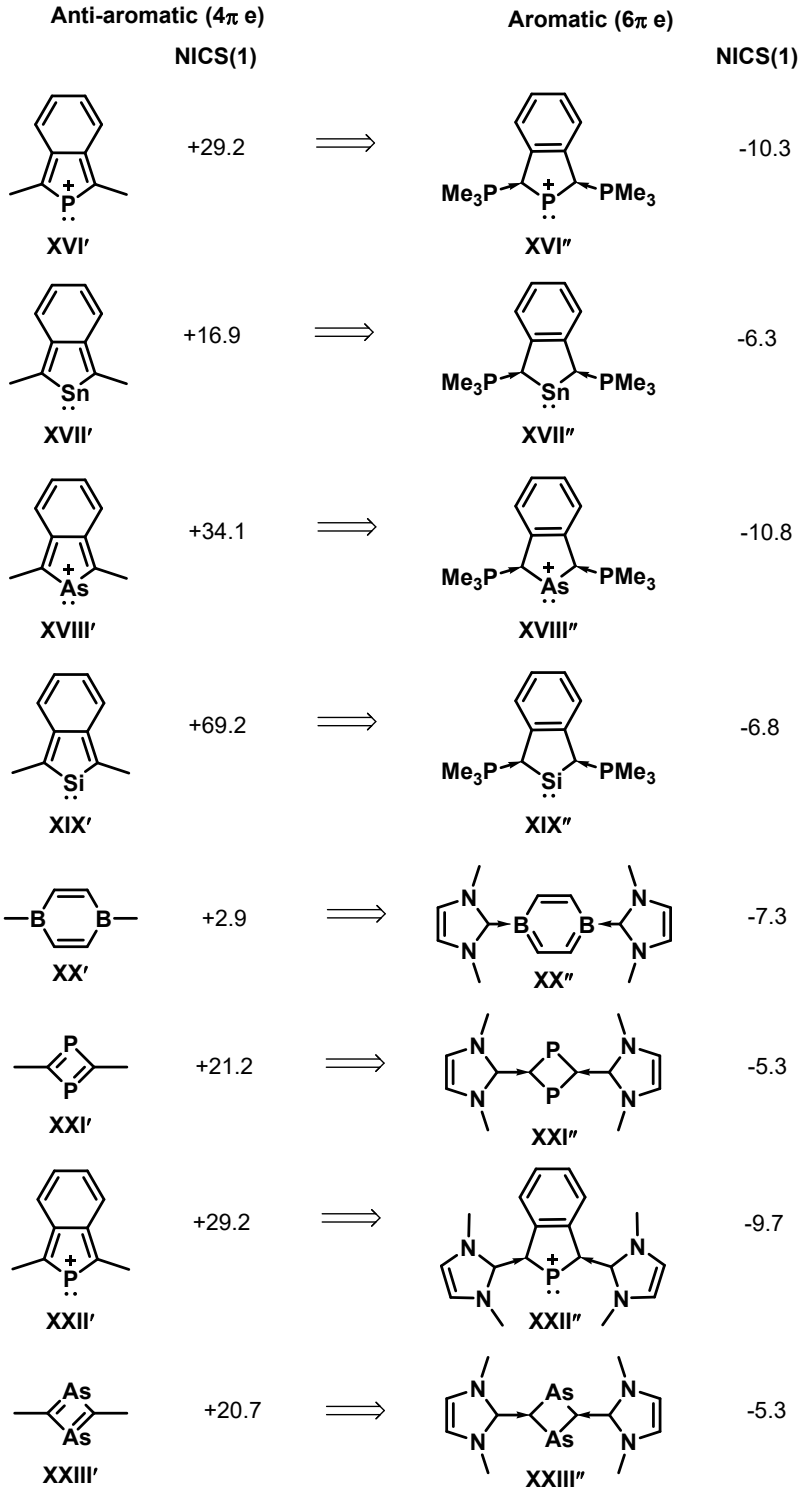
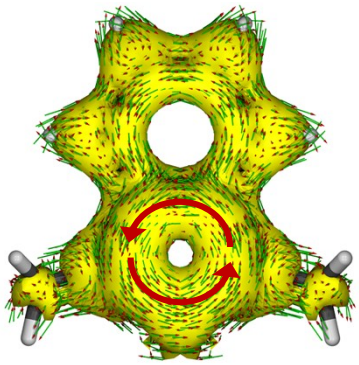
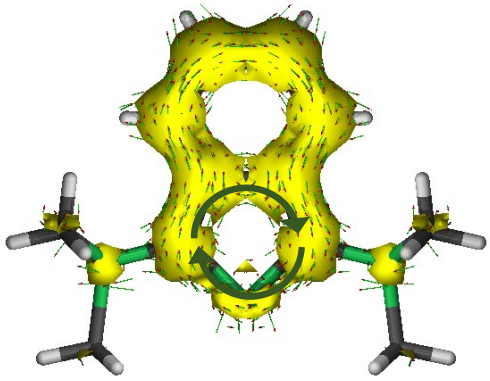


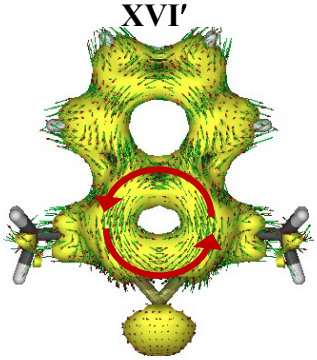
Figure S9. Schematic diagram showing anti-aromatic rings (**XVI′- XXIII′**) gain aromatic character upon replacing Me group with NHC ligand (**XVI″- XXIII″**) respectively, along with the comparison of NICS values. The complete optimization of **XVII′** gave non planar tricyclic ring with additional C-C bond.



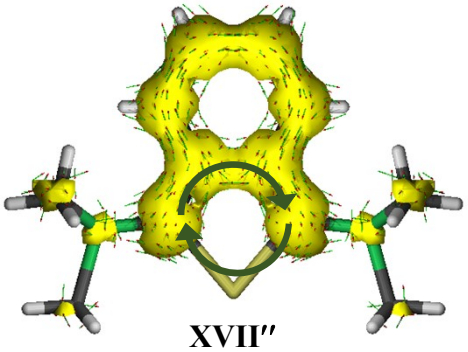
XVI′



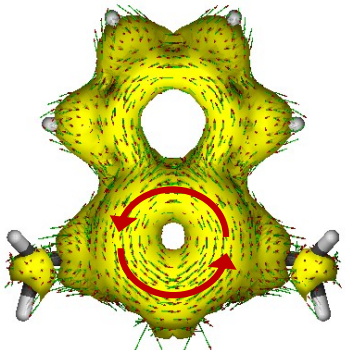
XVI″



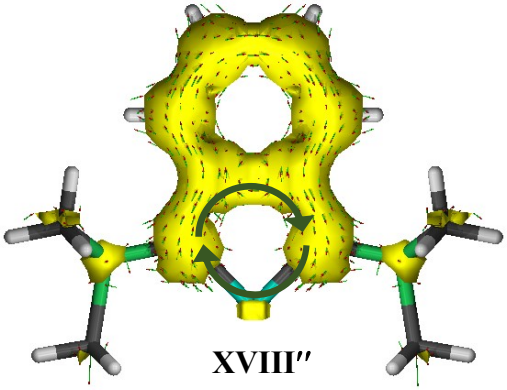
XVII′



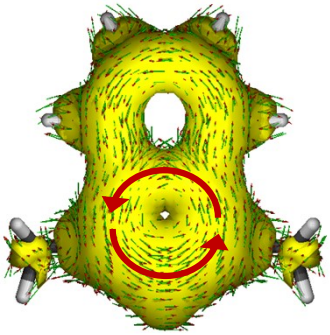
XVII″



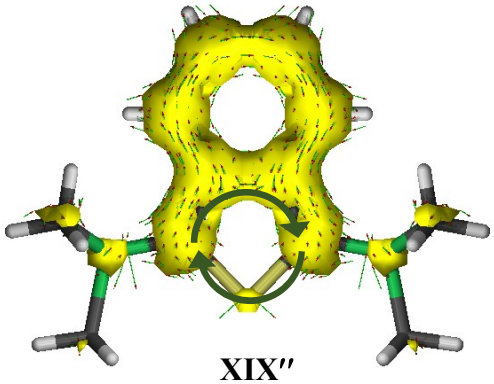
XVIII′



XVIII″



XIX′



XIX″

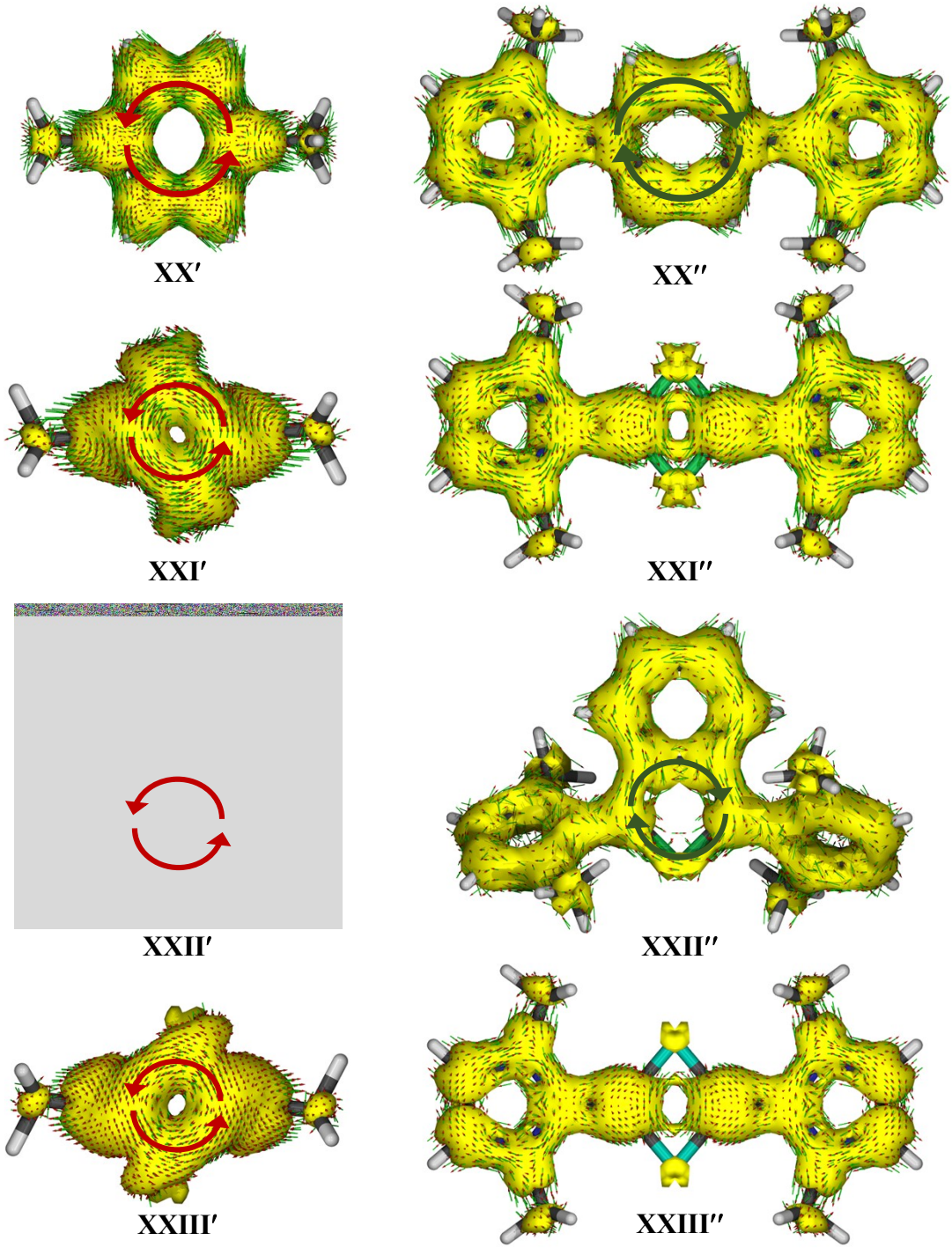


Figure S10. Contour diagrams generated for compounds (**XVI′- XXIII′** and **XVI″- XXIII″**) using ACID analysis. Clockwise direction of arrows indicates aromatic character in the ring while anticlockwise depicts anti-aromatic character.

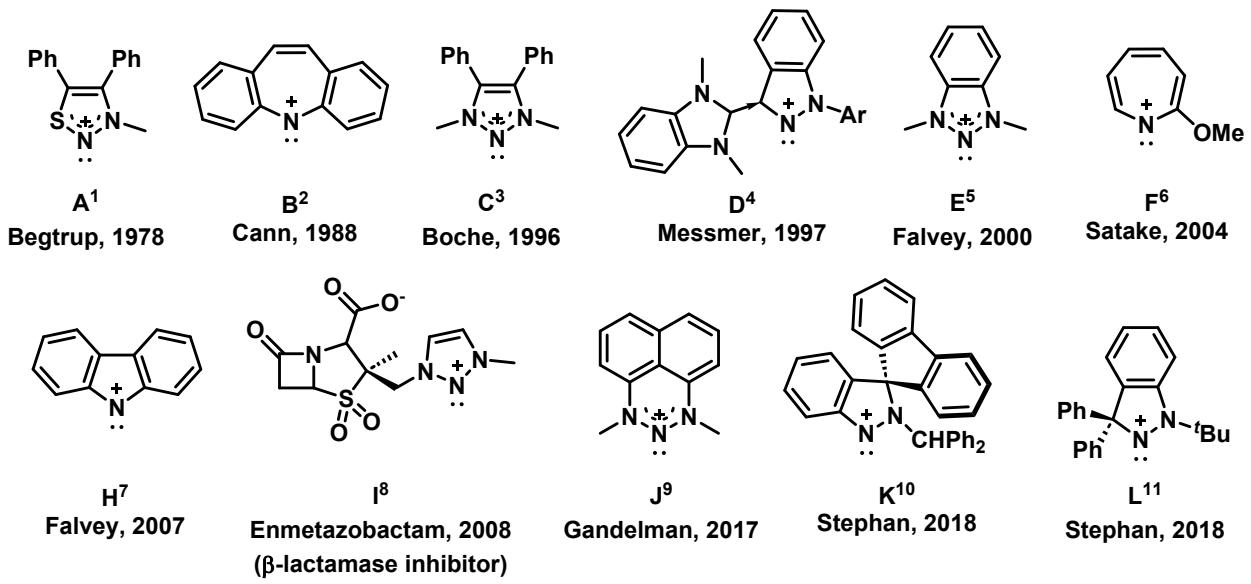
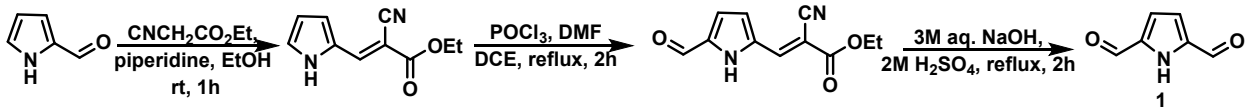


Figure S11. Experimentally known Cyclic Nitrenium ions (**A**-**L**).[2-12]

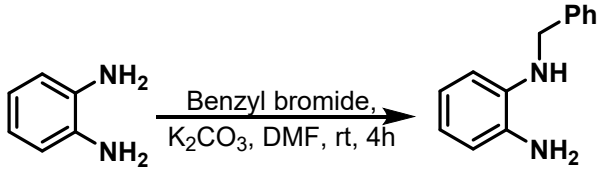
EXPERIMENTAL SECTION

Scheme S1. Preparation of Compound 1.[13]



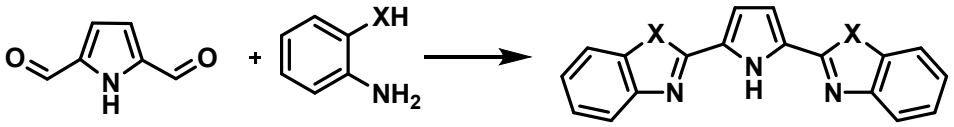
To a solution of pyrrole-2-carboxaldehyde (2.5 g, 26 mmol) and ethyl cyanoacetate (3.5 g, 32 mmol) in 50 ml of ethanol, the catalytic amount of piperidine was added. The reaction was stirred for 1 hour at room temperature. After the given time, the precipitates were formed. These precipitates were filtrated and washed by petroleum ether to afford 4.0 g α-cyano-2-pyrroleacrylate (80 % yield). Further, in another reaction vessel, phosphoryl oxychloride (3.5 g, 23 mmol) in dichloroethane was added dropwise to a cooled solution of *N,N*-dimethylformamide (1.7 g, 23 mmol). The temperature during the addition was maintained at 0 C. The contents of the flask were warmed to rt and stirred for 15 mins. α-cyano-2-pyrroleacrylate (4.0 g, 21 mmol) in dichloroethane was added in a dropwise manner to the flask at 0 C. The ice bath was removed and the reaction mixture was allowed to reflux for 30 mins. The solution was cooled to rt and sodium acetate (8.7 g, 105 mmol) was added. The mixture was refluxed again for 20 mins and allowed to cool to rt. The precipitate formed was filtered to afford Ethyl α-cyano-5-formyl-2-pyrroleacrylate as 3.5 g greenish-brown powder (76 % yield). The alkaline hydrolysis of Ethyl α-cyano-5-formyl-2-pyrroleacrylate was carried out. Ethyl α-cyano-5-formyl-2-pyrroleacrylate (3.5 g, 16 mmol) was added to a 3M aqueous solution of NaOH (45 mL) and was allowed to reflux for 2 h. The mixture was then cooled to 20 °C and acidified with a 2M solution of H_2SO_4. The reaction mixture was extracted with ethyl acetate-water workup. Column chromatography was employed to get 1.6 g of pyrrole-2,5-dicarboxaldehyde in pure form for further reactions.

Scheme S2. Preparation of Compound 2c.[14]



K_2CO_3 (2.5 g, 18 mmol) and benzyl bromide (1.1 g, 6 mmol) was added to a solution of *o*-phenylenediamine (1 g, 9.3 mmol) in DMF (30 mL). The mixture was allowed to stir at room temperature for 5 h and then diluted with EtOAc (50 mL). The inorganic impurities were washed off by ethyl acetate-water workup. The organic layer was collected and dried over sodium sulfate and concentrated by using a rotary evaporator. The residual oil was purified by silica gel column chromatography using the solvent system: (ethyl acetate: hexane in 1:9 ratio).

Scheme S3: Preparation of Compound 3a-d.[15]



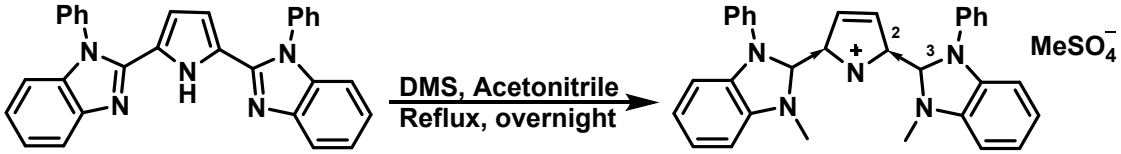
1 **2a-d** **3a-d**

2a, 3a: X = N-Ph
2b, 3b: X = N-Me
2c, 3c: X = N-Bz
2d, 3d: X = S

3a, Yield = 73 %
3b, Yield = 64 %
3c, Yield = 65 %
3d, Yield = 42 %

A solution of compound **2a** (122 mg, 1 mmol), **1** (123 mg, 0.5 mmol), iodine (23 mg, 0.15 mmol), UHP (24 mg, 0.25 mmol) in acetonitrile (5 mL) was stirred at 70 ºC for 4-5 hours. After completion of the reaction as indicated by TLC, the reaction mixture was cooled to rt. The inorganic impurities were washed off by ethyl acetate-water workup. The crude mass was purified by silica gel column chromatography using ethyl acetate: hexane (2:8) to afford the title compound **3a**. Compounds 3**b-d** were synthesized using similar procedure.

Scheme S4: Preparation of Compound 4a (salt). For the crystal structure of 4a, see Figure S4.



3a **4a**

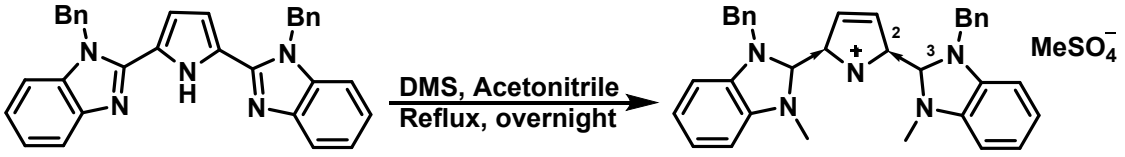
Compound **3a** (45 mg, 0.1 mmol) and dimethyl sulphate (100 mg, 0.8 mmol) were mixed together in 5-6 ml of acetonitrile solvent in a 10 ml round bottom flask. The reaction mixture was allowed to reflux (90-95 °C) for 12-14 hours. The reaction was monitored by using TLC. After cooling the reaction mixture to rt, the remaining solvent was removed under reduced pressure

and neutralized with Na_2CO_3 solution. The aqueous phase was extracted with dichloromethane. The title compound **4a** was obtained from the organic layer by preparative TLC taking MeOH:EtOAc as a solvent in the ratio of 1:9, v/v. The pure title compound was obtained in 44 % isolated yield. It is pertinent to add that it is possible to isolate the dicationic species before treating it with base.

Scheme S5: Preparation of Compound 4b

Compound **3b** (33 mg, 0.1 mmol) and methyl triflate (49 mg, 0.3 mmol) were mixed together in 4 ml of dichloromethane solvent in a 10 ml round bottom flask. The reaction mixture was allowed to stir at 0 °C for 2-3 hours. The reaction was monitored by TLC. After thawing the reaction mixture to rt, the remaining solvent was removed under reduced pressure. The reaction mixture was neutralized with triethylamine. The title compound **4b** was obtained from the organic layer by preparative TLC. The pure title compound was obtained in 64 % isolated yield.

Scheme S6: Preparation of Compound 4c



3c **4c**

Compound **3c** (20 mg, 0.04 mmol) and dimethyl sulphate (41 mg, 0.32 mmol) were mixed together in 5 ml of acetonitrile in a 5 ml round bottom flask. The reaction mixture was allowed to reflux for 12-14 hours. The reaction was monitored by TLC. After cooling the reaction mixture to rt, the remaining solvent was removed under reduced pressure and neutralized with Na_2CO_3 solution. The aqueous phase was extracted with dichloromethane. The title compound **4c** was purified by preparative TLC taking MeOH: EtOAc as a solvent in the ratio of 1:9 v/v. The pure title compound was obtained in 25 % isolated yield.

Scheme S7: Preparation of Compound 4d

3d 4d

Compound **3d** (10 mg, 0.03 mmol) and methyl triflate (15 mg, 0.09 mmol) were mixed together in 5 ml dichloromethane solvent in a 10 ml round bottom flask. The reaction mixture was allowed to sir at 0 °C for 2-3 hours. The reaction was monitored by using TLC. After thawing the reaction mixture to rt, the remaining solvent was removed under reduced pressure. The title compound **4d** was purified by washing with dichloromethane and diethyl ether subsequently to afford the final product. The pure title compound was obtained in 23% isolated yield.

Spectral Data:

Compound 1: Pinkish-brown solid; 46 % overall yield; ^{1}H NMR (Chloroform-*d*): δ = 10.45 (br s, 1H), 9.77 (s, 2H), 7.01 (s, 2H).

Compound 2c: Dark brown viscous liquid; 67 % overall yield. ^{1}H NMR (Chloroform-*d*): δ = 7.35 (m, 5H), 6.76 (m, 4H), 4.32 (s, 2H), 3.43 (s, 3H).

Compound 3a: Yellow solid; overall yield 325 mg, 73 %; M.P.: 234-236 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ: 10.74 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.56 (dd, *J* = 5.1, 2.1 Hz, 6H), 7.41 (dd, *J* = 7.4, 2.2 Hz, 4H), 7.31 (t, *J* = 7.0 Hz, 2H), 7.21 (t, *J* = 7.0 Hz,2H), 7.03 (d, *J* = 8.0 Hz, 2H), 5.41 (s, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ: 145.61, 143.05, 137.74, 136.53, 130.16, 129.64, 128.37, 124.18, 123.09, 123.02, 119.22, 111.38, 110.03, 77.36, 77.15, 76.93, 0.12; HRMS-ESI *m/z* calcd for $C_{30}H_{22}N_5^+$ [M+H$^+$] 452.1870, found 452.1877.

Compound 3b: Pale white solid; overall yield 208 mg, 64 %; M.P.: 296-298 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ: 11.77 (s, 1H), 7.61 (dd, *J* = 21.2, 7.8 Hz, 4H), 7.27 – 7.18 (m, 4H), 6.97 (s, 2H), 3.98 (s, 6H); ^{13}C NMR (151 MHz, DMSO-d_6) δ: 146.69, 142.90, 136.87, 124.66, 122.70, 122.55, 119.06, 112.77, 110.77, 40.46, 40.32, 40.18, 40.04, 39.91, 39.77, 39.63, 31.91; LCMS-ESI *m/z* calcd for $C_{20}H_{18}N_5^+$ [M+H$^+$] 327.15, found 327.90.

Compound 3c: Light brown solid; overall yield 310 mg, 65 %; M.P.: 246-249 °C; ^{1}H NMR (500 MHz, Chloroform-*d*) δ: 7.82 (dd, *J* = 8.0, 1.0 Hz, 2H), 7.35 – 7.26 (m, 8H), 7.24 (d, *J* = 5.7 Hz, 4H), 7.10 (d, *J* = 6.5 Hz, 4H), 6.41 (s, 2H), 5.58 (s, 4H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ: 146.14, 142.91, 136.33, 135.97, 129.26, 127.93, 125.92, 124.06, 123.13, 123.06, 119.53, 111.45, 109.75, 77.38, 77.13, 76.87, 48.10; HRMS-ESI *m/z* calcd for $C_{32}H_{26}N_5^+$ [M+H$^+$] 480.2183, found 480.2196.

Compound 3d: Yellow solid; overall yield 140 mg, 42 %; M.P.: 205-207 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 10.52 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.48 (t, *J* = 7.0 Hz, 2H), 7.35 (t, 2H), 6.89 (d, *J* = 1.7 Hz, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ: 158.57, 153.74, 134.46, 129.37, 126.59, 122.67, 121.66, 113.50, 113.42, 77.34, 77.13, 76.91, 0.10; HRMS-ESI *m/z* calcd for $C_{18}H_{11}N_3S_2^+$ [M$^+$] 334.0467, found 334.0468.

Compound 4a: Bright yellow solid; overall yield 35 mg, 44 %; M.P.: 202-205 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ: 7.85 (d, *J* = 8.2 Hz, 2H), 7.67 – 7.62 (m, 6H), 7.56 (t, 2H), 7.44 –

7.39 (m, 6H), 7.08 (d, *J* = 8.1 Hz, 2H), 5.79 (s, 2H), 4.51 (s, 6H), 3.71 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ: 147.08, 134.76, 133.19, 132.80, 130.97, 130.88, 128.70, 127.99, 126.44, 126.22, 119.23, 112.45, 111.73, 77.34, 77.13, 76.92, 54.38, 35.01; HRMS-ESI *m/z* calcd for $C_{32}H_{26}N_5^+$ [M^+] 480.2183, found 480.2225.

Compound 4b: White solid; overall yield 48 mg, 64 %; M.P.: 290-293 °C; ^{1}H NMR (600 MHz, Methanol-d_4) δ: 8.02 (dd, *J* = 6.2, 3.2 Hz, 4H), 7.79 (dd, *J* = 6.3, 3.1 Hz, 4H), 7.39 (s, 2H), 4.16 (s, 12H); ^{13}C NMR (151 MHz, Methanol-d_4) δ: 144.28, 133.77, 128.86, 120.43, 118.34, 114.33, 54.85, 49.48, 49.34, 49.20, 49.05, 48.91, 48.76, 48.62, 33.85; HRMS-ESI *m/z* calcd for $C_{22}H_{22}N_5^+$ [M^+] 356.1870, found 356.1891.

Compound 4c: Pale Yellow solid; overall yield 7 mg, 25 %; ^{1}H NMR (600 MHz, Chloroform-*d*) δ: 7.75 (d, *J* = 8.2 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 7.2 Hz, 6H), 7.16 (d, *J* = 5.6 Hz, 4H), 5.96 (s, 4H), 4.27 (s, 6H), 3.68 (s, 3H). HRMS-ESI *m/z* calcd for $C_{34}H_{30}N_5^+$ [M^+] 508.2496, found 508.2518.

Compound 4d: Fluorescent yellow solid; overall yield 8 mg, 23 %; ^{1}H NMR (600 MHz, Methanol-d_4) δ: 8.27 (t, *J* = 9.4 Hz, 2H), 8.20 (t, *J* = 9.4 Hz, 2H), 7.89 (q, *J* = 8.7, 8.0 Hz, 2H), 7.78 (q, *J* = 9.2, 8.5 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 2H), 4.52 (s, 6H); HRMS-ESI *m/z* calcd for $C_{20}H_{16}N_3S_2^+$ [M^+] 362.0780, found 362.0811.

Spectroscopic data for synthesized compounds:

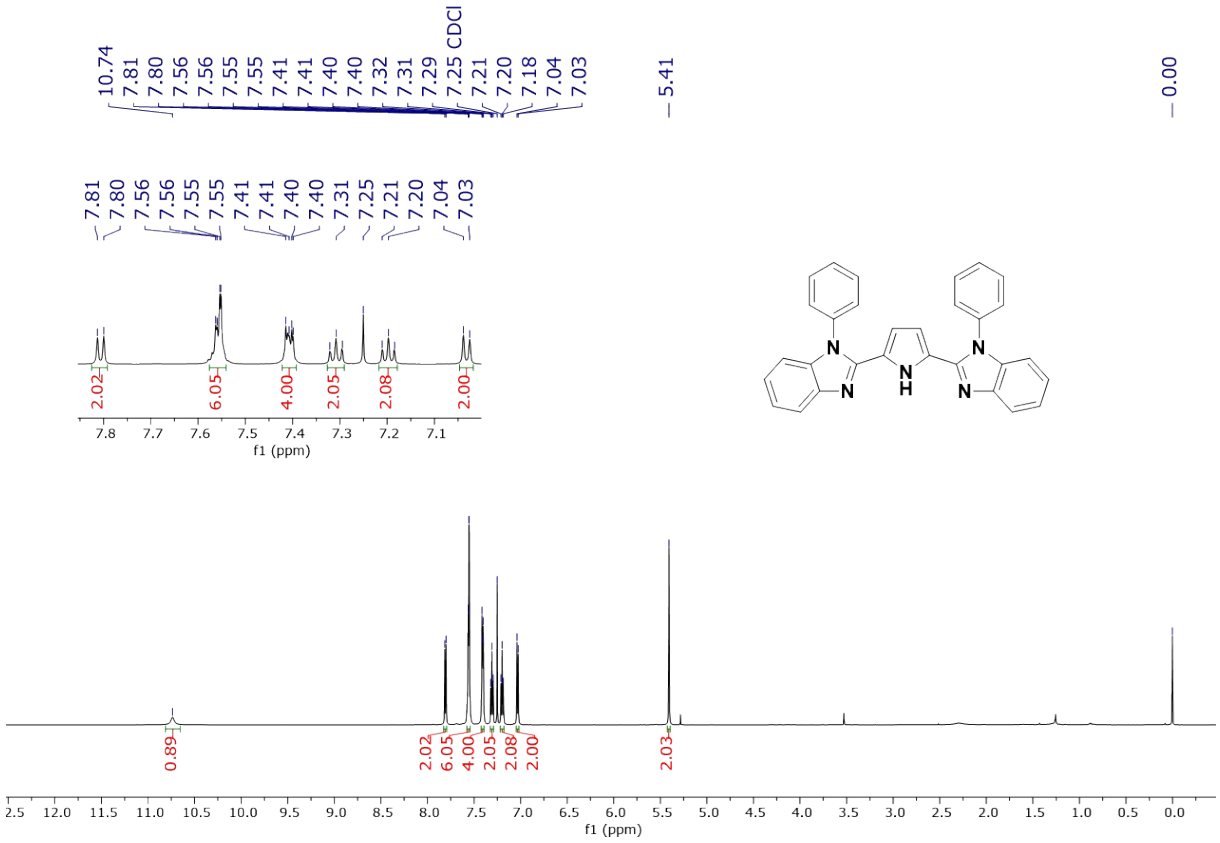


Figure S12. ^{1}H NMR spectrum of **3a** at 600 MHz in $CDCl_3$ at 298K

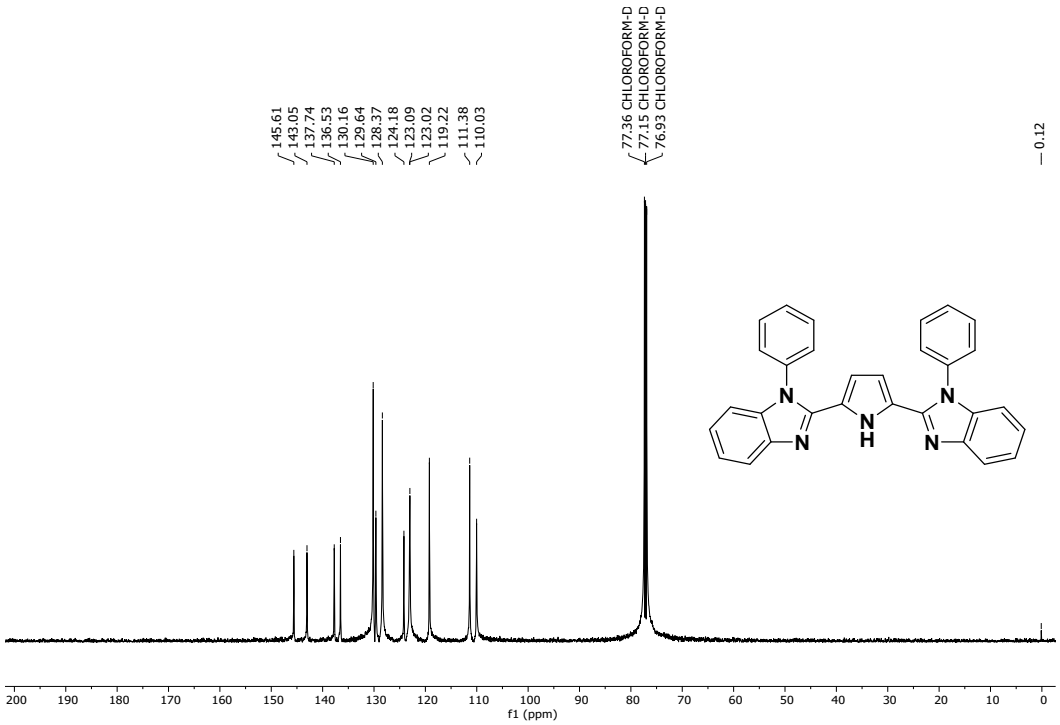
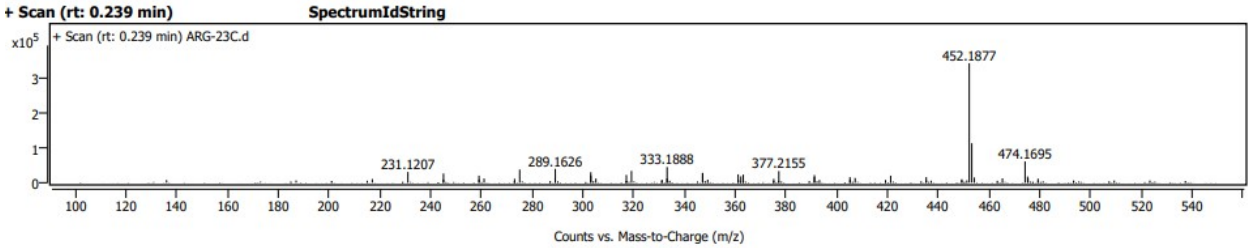


Figure S13. ^{13}C NMR spectrum of **3a** at 151 MHz in $CDCl_3$ at 298K



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
231.1207		30633	8.93					
275.1472		37792	11.02					
289.1626		39784	11.60					
303.1421		30097	8.77					
319.1732		33971	9.90					
333.1888		44990	13.12					
377.2155		33452	9.75					
452.1877	1	343041	100.00					
453.1910	1	113299	33.03					
474.1695		61215	17.84					

Figure S14. HRMS of **3a** in ESI (+) mode

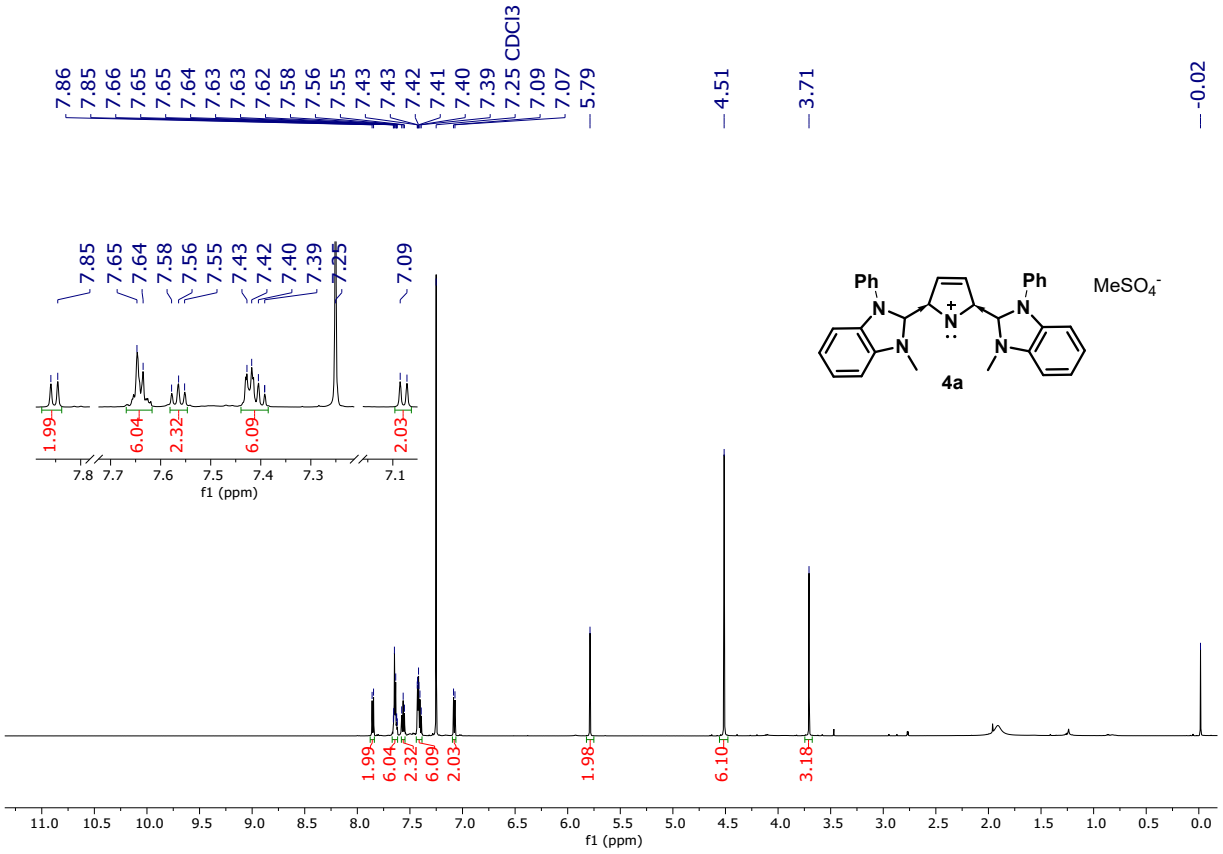


Figure S15. ^{1}H NMR spectrum of **4a** at 600 MHz in $CDCl_3$ at 298K

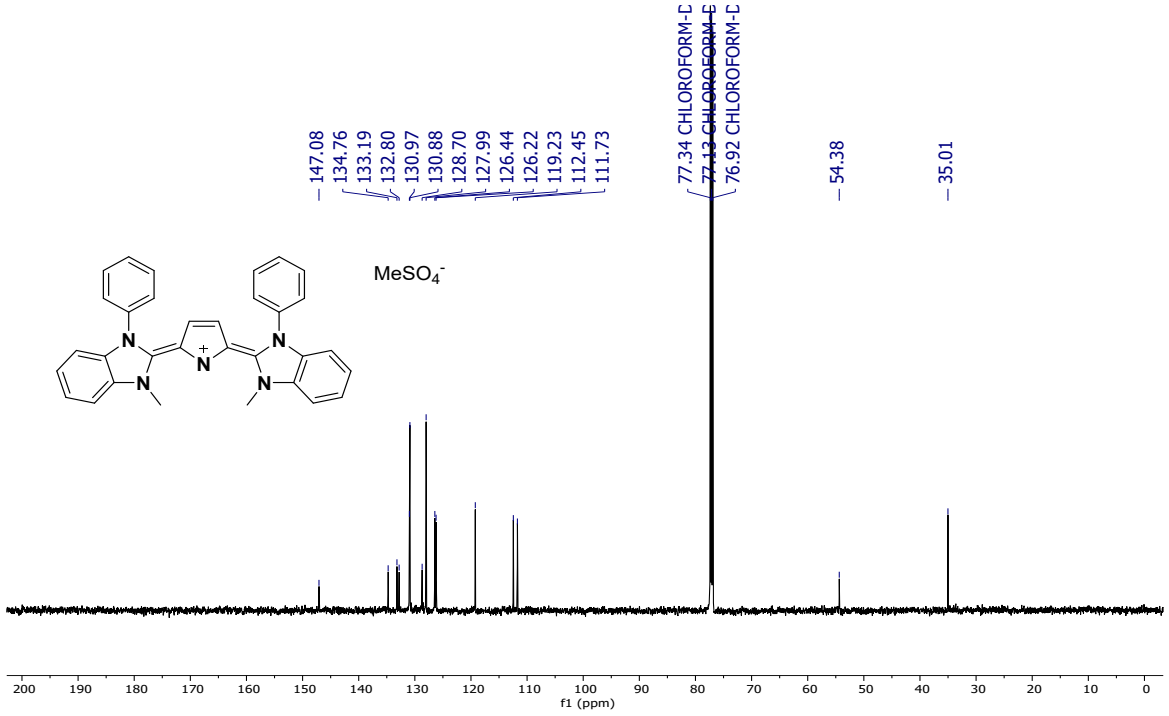
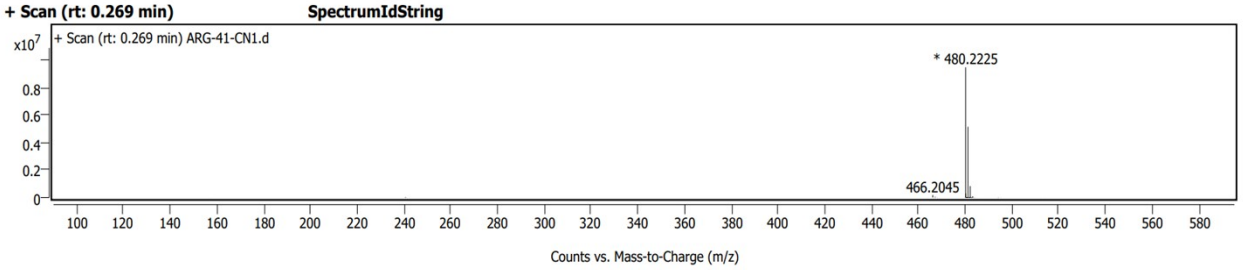
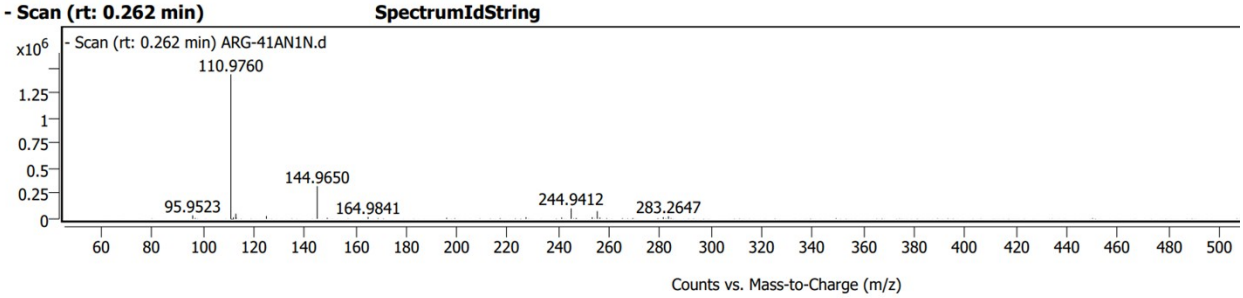


Figure S16. ^{13}C NMR spectrum of **4a** at 151 MHz in $CDCl_3$ at 298K



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
466.2045		176627	1.85					
480.2225	1	9522580	100.00					
480.3333		293287	3.08					
481.2251	1	5174426	54.34					
482.2268	1	834468	8.76					
483.2297	1	95770	1.01					



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	I
95.9523		36157	2.51					
110.9760	1	1442350	100.00					
111.9784	1	16117	1.12					
112.9715	1	52693	3.65					
124.9915		29443	2.04					
144.9650		327111	22.68					
164.9841		19231	1.33					
227.2021		16674	1.16					
244.9412		104366	7.24					
253.2179		16606	1.15					
255.2338		77607	5.38					
281.2488		16924	1.17					
283.2647		26888	1.86					

Figure S17. HRMS of **4a** in ESI (+) mode and ESI (-) mode

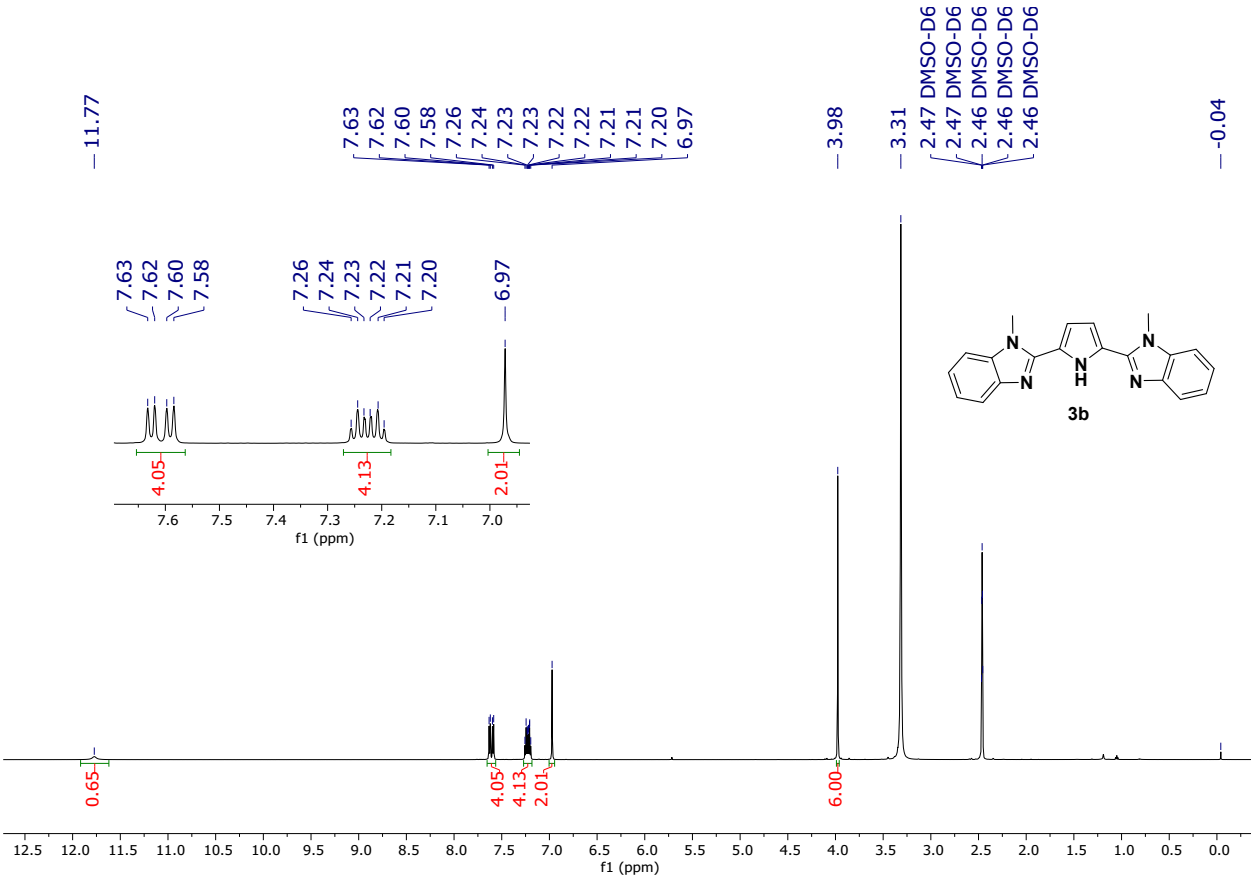


Figure S18. ^{1}H NMR spectrum of **3b** at 600 MHz in DMSO-d_6 at 298K

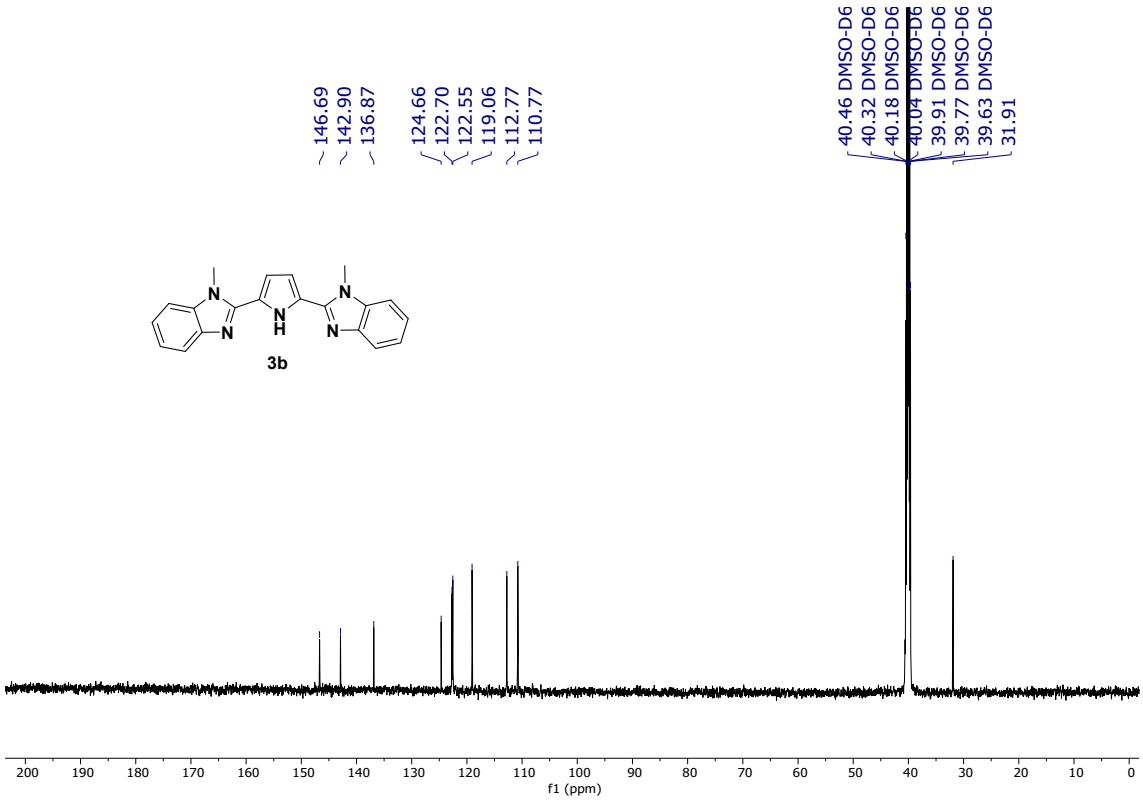


Figure S19. ^{13}C NMR spectrum of **3b** at 150 MHz in DMSO-d_6 at 298K

Figure S20. LCMS of **3b** in ESI (+) mode

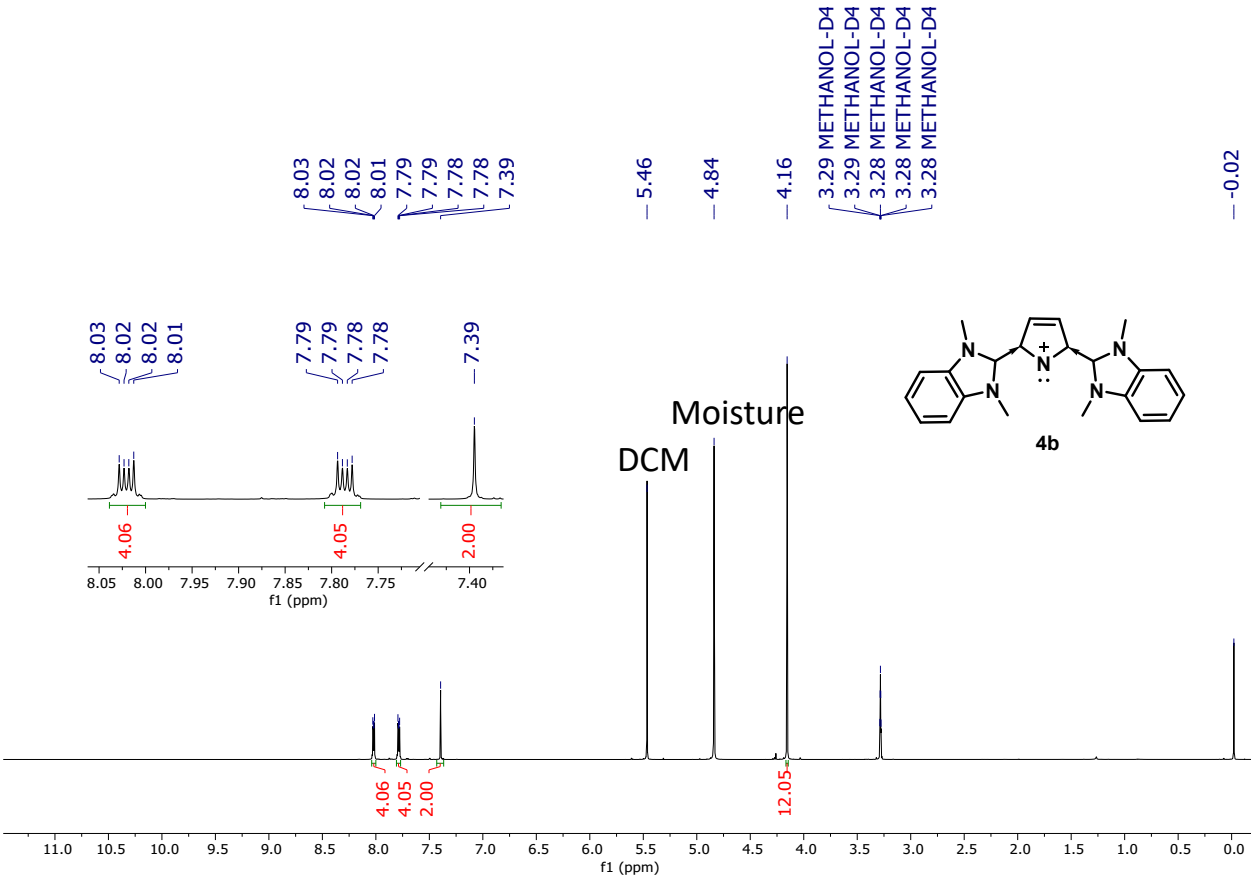


Figure S21. ^{1}H NMR spectrum of **4b** at 600 MHz in Methanol-d_4 at 298K

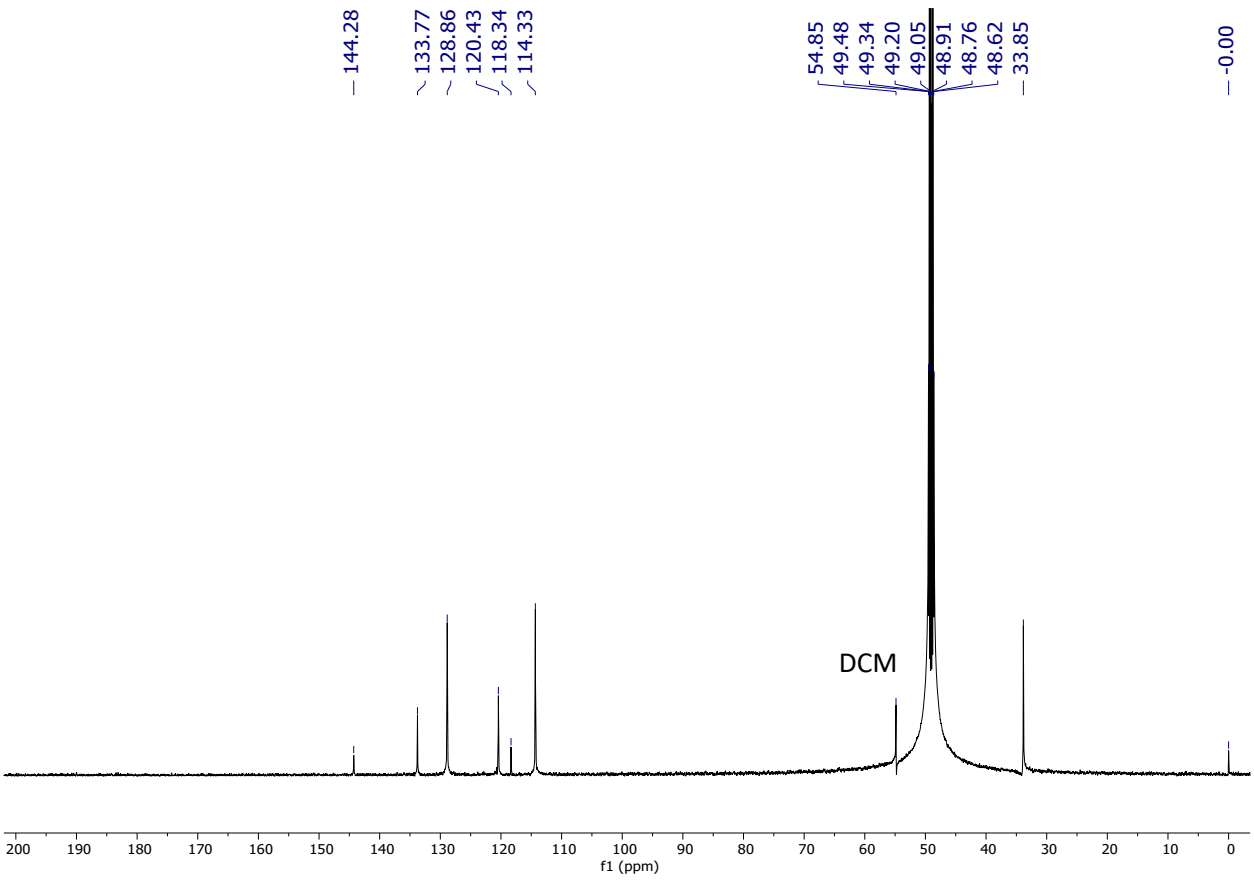
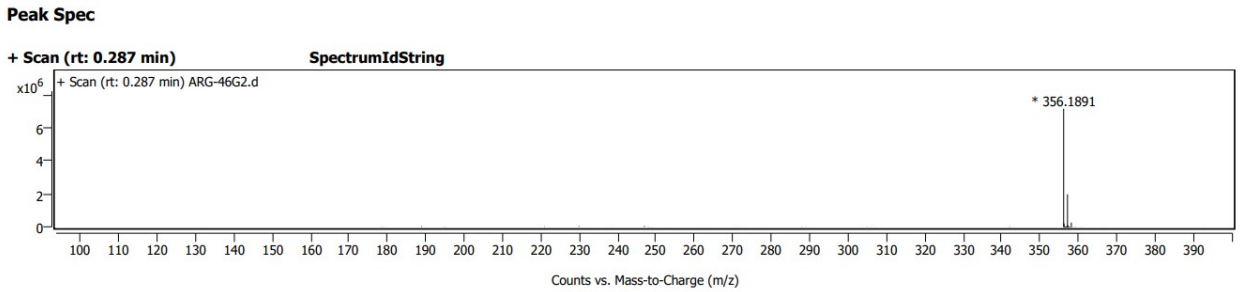


Figure S22. ^{13}C NMR spectrum of **4b** at 151 MHz in Methanol-d_4 at 298K



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
356.1891	1	7166318	100.00					
356.2849		202885	2.83					
357.1911	1	1971114	27.51					
357.2139		81779	1.14					
357.2333		80092	1.12					
358.1940	1	256736	3.58					

Figure S23. HRMS of **4b** in ESI (+) mode

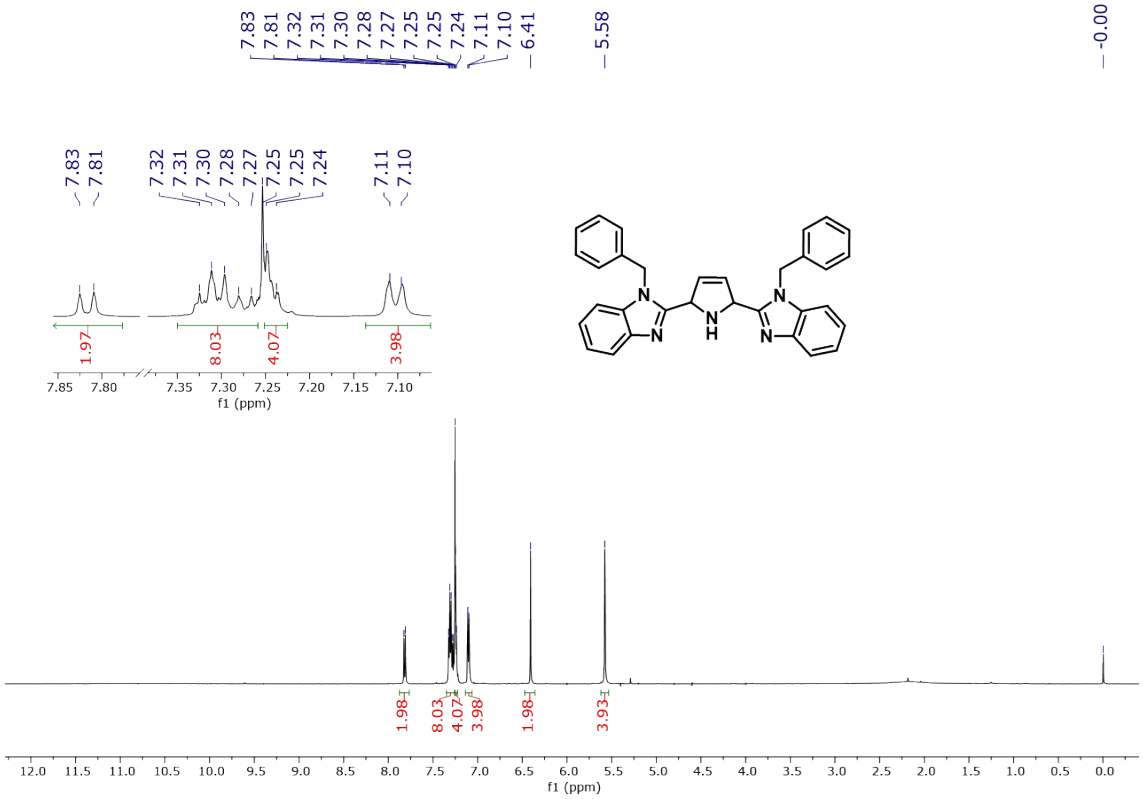


Figure S24. ^{1}H NMR spectrum of **3c** at 600 MHz in $CDCl_3$ at 298K

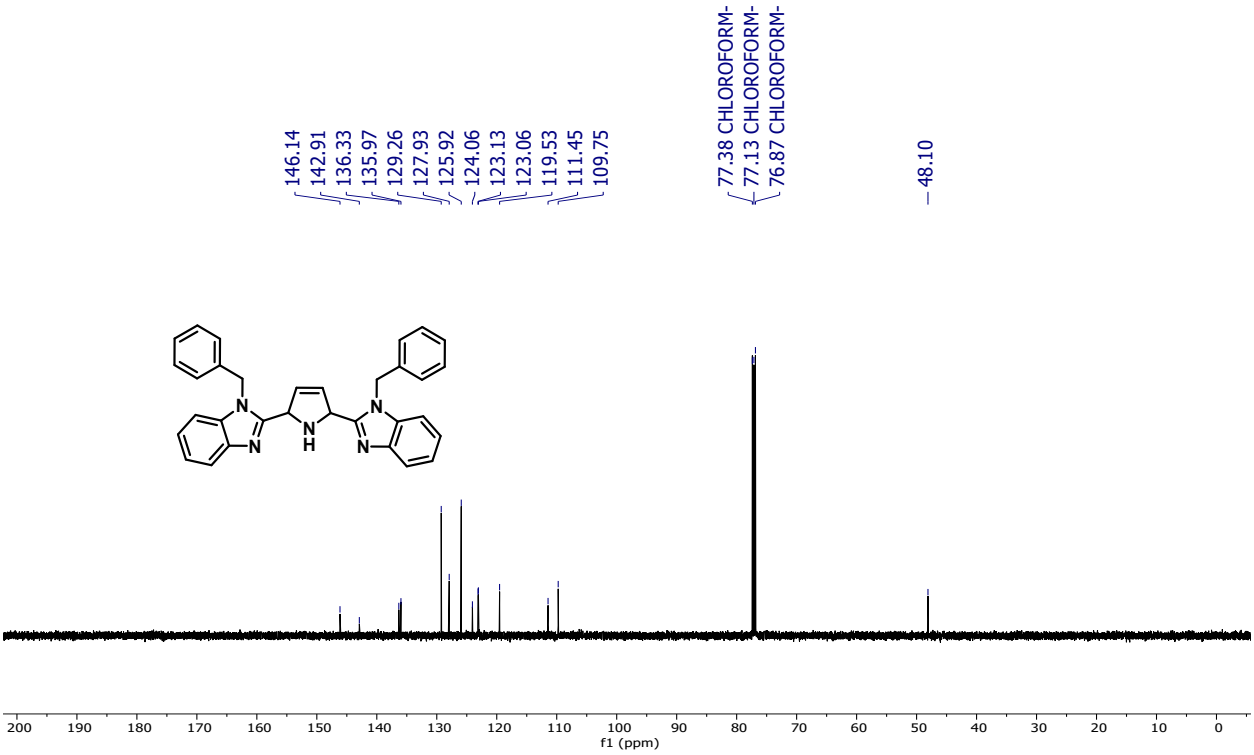
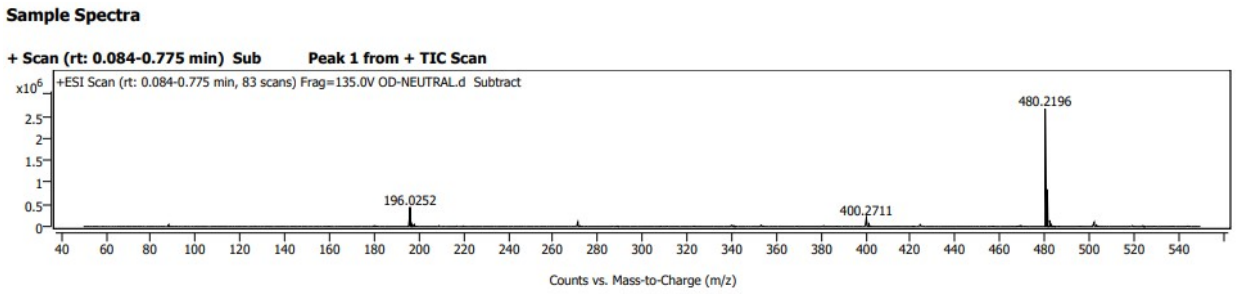


Figure S25. ^{13}C NMR of **3c** at 151 MHz in $CDCl_3$ at 298K



Spectrum Peaks

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
196.0252		440557	16.39					
400.2711		204961	7.62					
480.2196	1	2688771	100.00					
481.2222	1	866263	32.22					
482.2251	1	140647	5.23					

Figure S26. HRMS of **3c** in ESI (+) mode

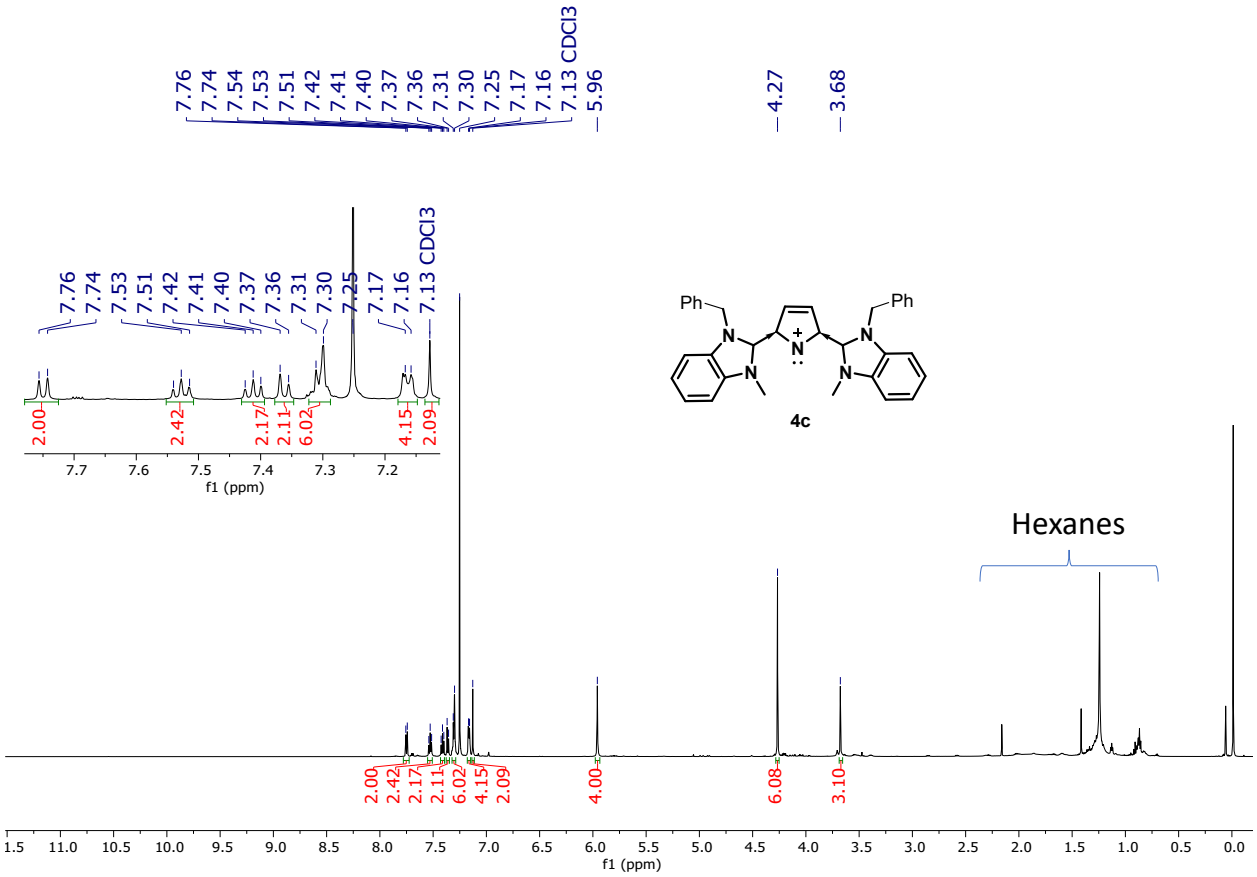
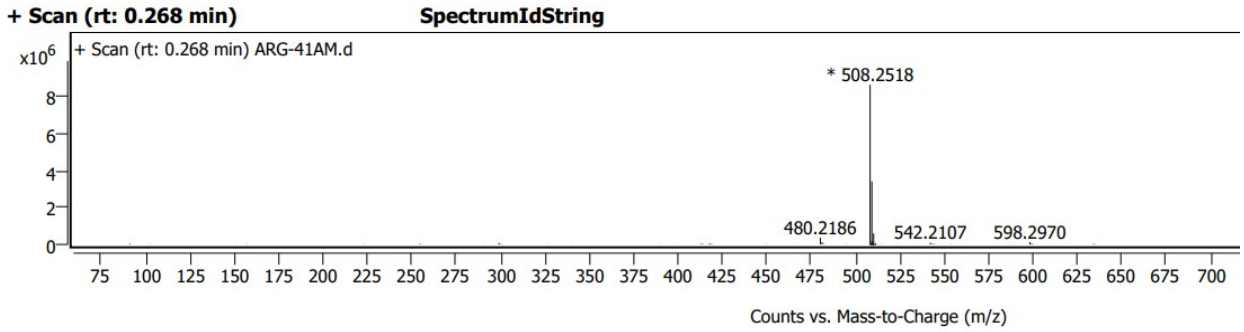


Figure S27. ^{1}H NMR spectrum of **4c** at 600 MHz in $CDCl_3$ at 298K



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
480.2186	1	365730	4.21				
481.2216	1	118175	1.36				
508.2518	1	8686593	100.00				
509.2538	1	3436047	39.56				
509.2768		185026	2.13				
510.2562	1	595958	6.86				
542.2107		90864	1.05				
598.2970		126177	1.45				

Figure S28. HRMS of **4c** in ESI (+) mode

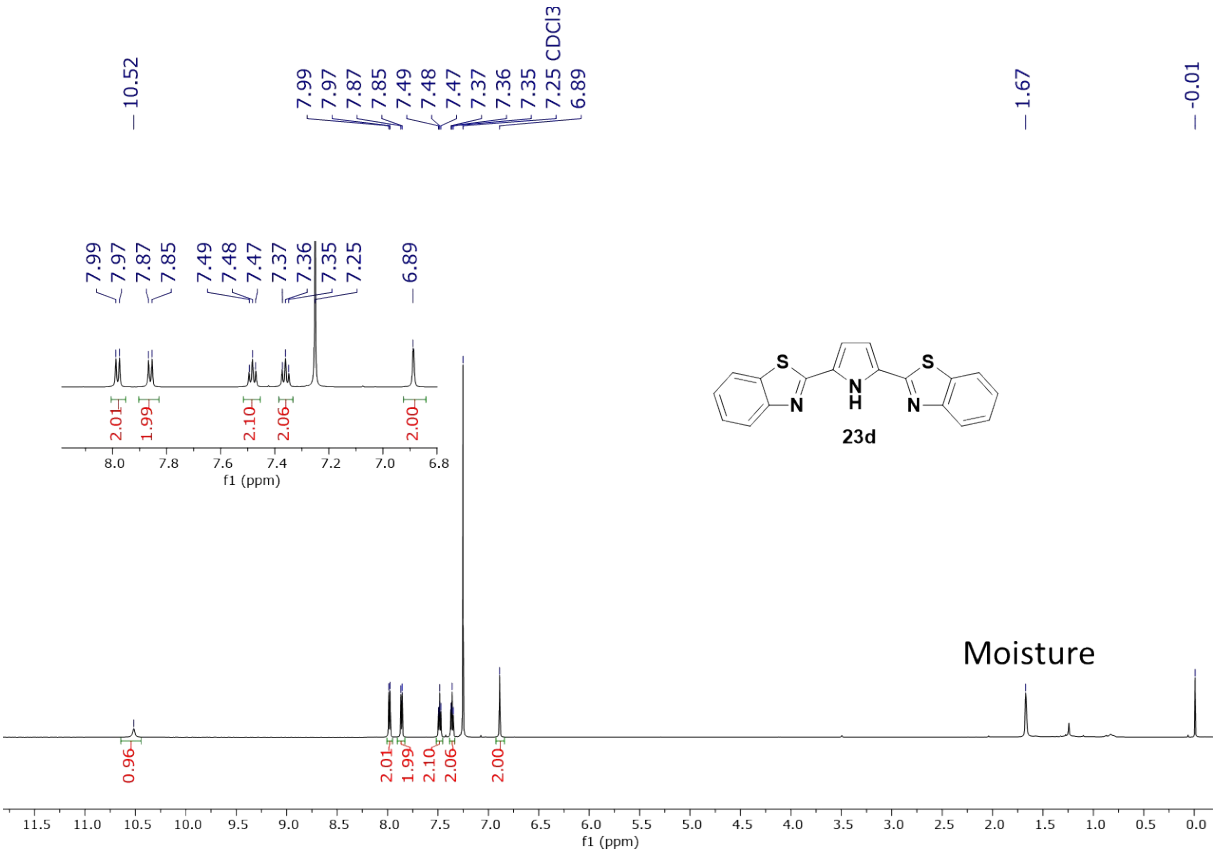


Figure S29. ^{1}H NMR spectrum of **3d** at 600 MHz in $CDCl_3$ at 298K

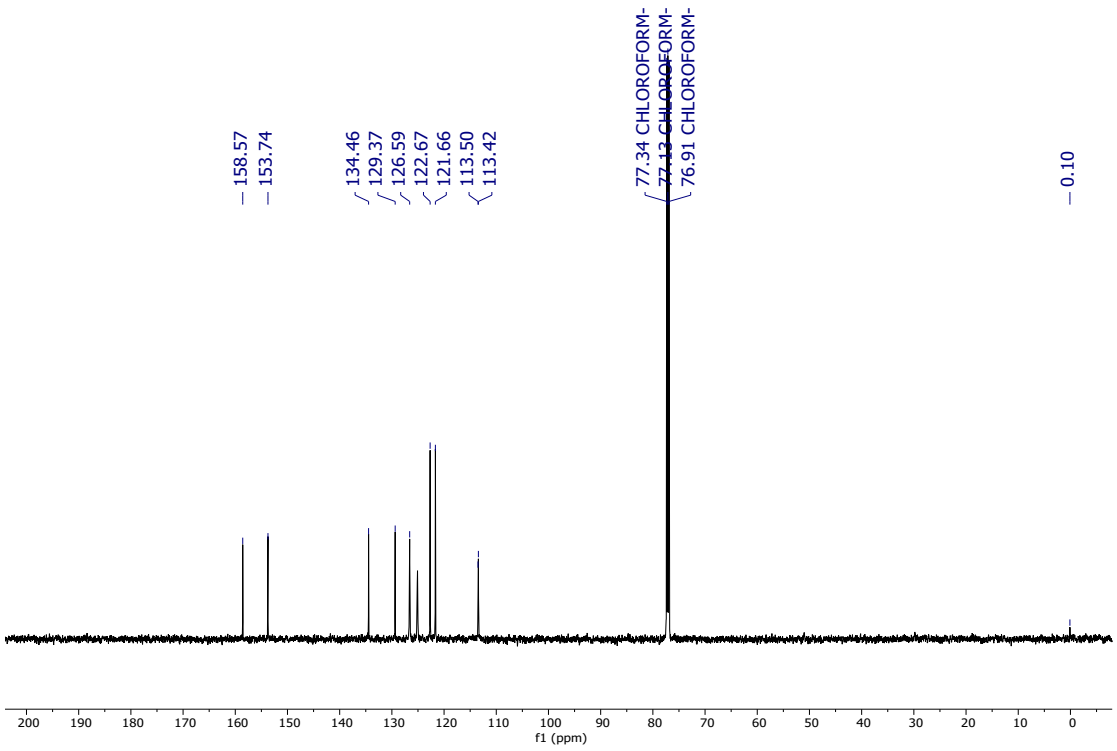
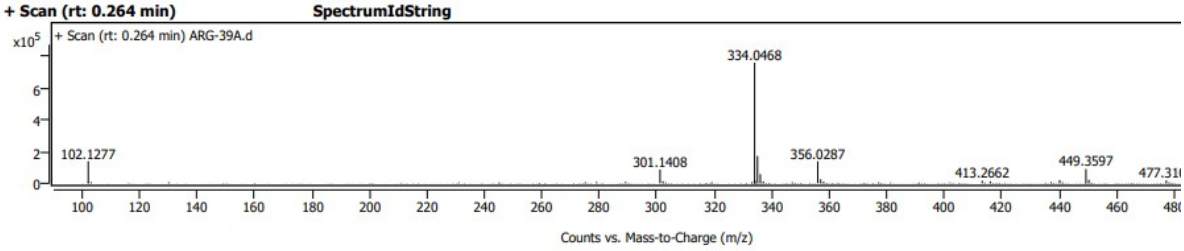


Figure S30. ^{13}C NMR spectrum of **3d** at 150 MHz in $CDCl_3$ at 298K

Peak Spec

+ Scan (rt: 0.264 min) **SpectrumIdString**



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
102.1277		139821	18.32					
102.1343		8288	1.09					
289.1621		9470	1.24					
301.1408	1	86609	11.35					
302.1444	1	13651	1.79					
333.1882		8736	1.14					
334.0468	1	763300	100.00					
334.1414		17798	2.33					
335.0497	1	172811	22.64					
336.0436	1	58423	7.65					
337.0468		12369	1.62					
356.0287	1	139020	18.21					
357.0313	1	25494	3.34					
358.0252	1	10801	1.42					
413.2662		16344	2.14					
416.0881		12236	1.60					
440.2195		20614	2.70					
449.3597	1	90409	11.84					
450.3630	1	23015	3.02					
477.3106		18539	2.43					

Figure S31. HRMS of **3d** in ESI (+) mode

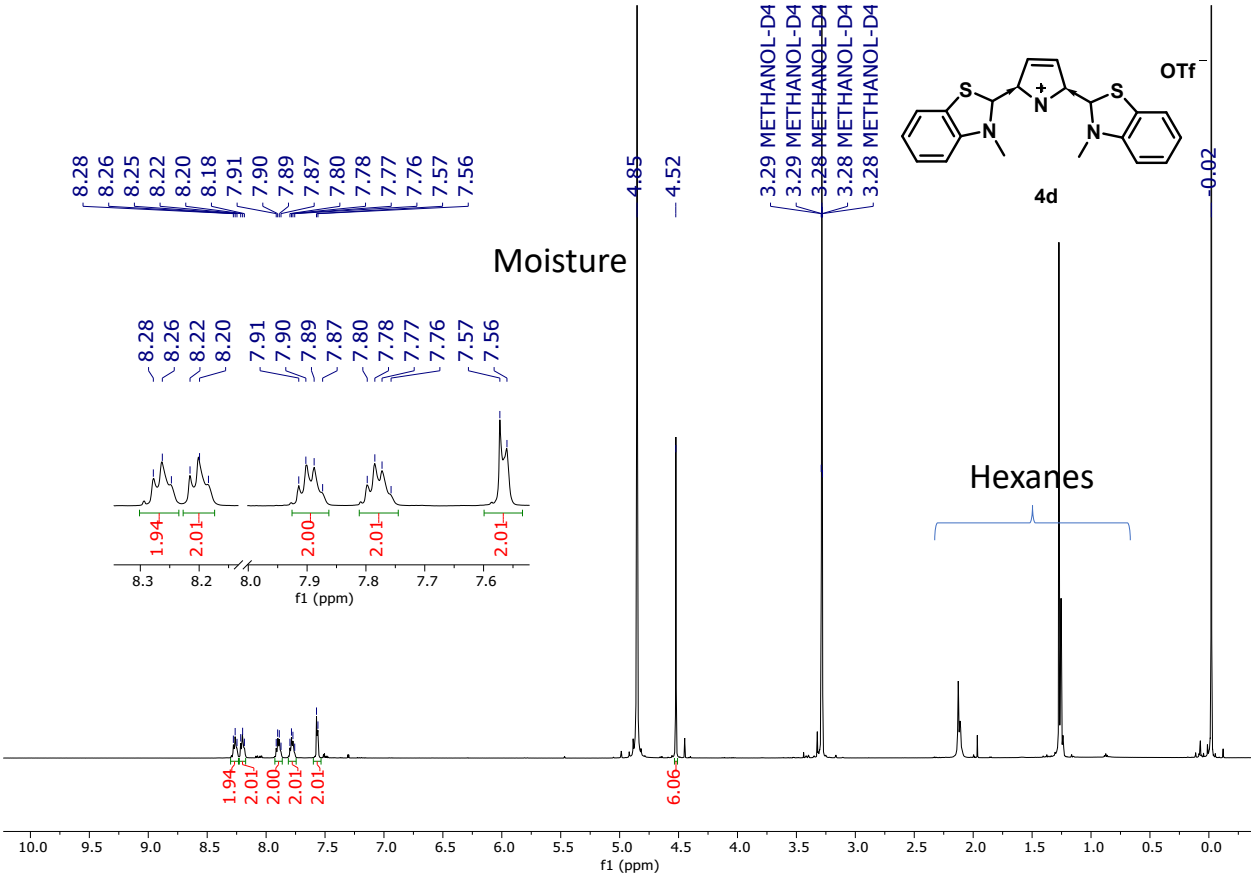
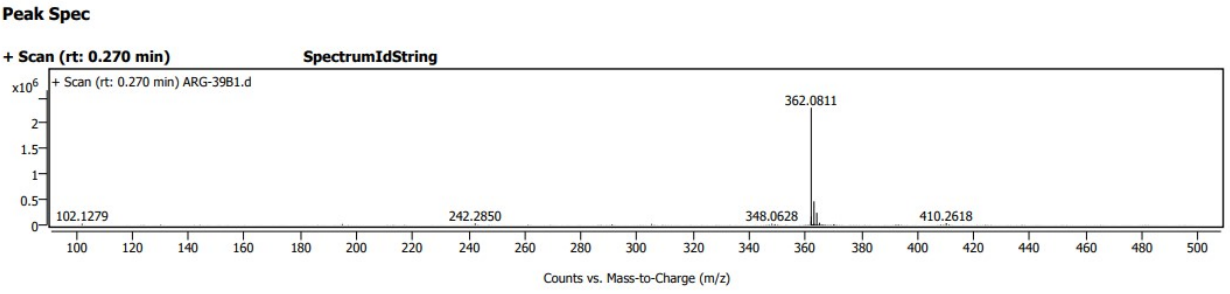


Figure S32. ^{1}H NMR spectrum of **4d** at 600 MHz Methanol-d_4 at 298K. Only 1H NMR could be generated as we got very less compound in hand.



SpectrumIdString

m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
102.1279		24630	1.07					
242.2850		29943	1.30					
348.0628		24509	1.06					
362.0483		69955	3.03					
362.0811	1	2309869	100.00					
362.1096		167677	7.26					
363.0831	1	466675	20.20					
364.0783	1	240768	10.42					
365.0788		43922	1.90					
410.2618		36145	1.56					

Figure S33. HRMS of **4d** in ESI (+) mode

Crystallographic Details:

The CrysAlisPro software was used for data acquisition and data extraction. Using OLEX2,[16] the structures were solved with the SIR2004[17] structure solution program using direct methods and refined with the SHELXL[18] refinement package using Least Squares minimization. All non-hydrogen atoms were refined with anisotropic thermal parameters. In the ORTEP diagram, ellipsoids were set at 50 % probability. The data was collected at room temperature and methyl sulphate anion in the unit cell was found to be disordered. An appropriate disordered treatment model was applied and hydrogens of the water molecule were omitted while the disorder treatment. Detailed crystallographic data and structural refinement parameters are summarized in Table S5-S8 Deposition Number CCDC2299060 contains the supplementary crystallographic data for this paper. The data are provided free of charge by the Cambridge Crystallographic Data Centre. http://www.ccdc.cam.ac.uk/services/structures.

Table S5. Crystal data and structure refinement for Compound **4a**

Identification code	ex-nipphe_autored
Empirical formula	$C_{33}H_{26}N_5O_7S$
Formula weight	636.670
Temperature/K	222.15
Crystal system	triclinic
Space group	P-1
a/Å	11.0277(5)
b/Å	12.5158(4)
c/Å	13.0402(5)
α/°	72.121(4)
β/°	65.597(4)
γ/°	88.754(3)
Volume/Å^3	1548.36(13)
Z	2
ρ_{calc}g/cm^3	1.366
μ/mm^{-1}	0.162
F(000)	662.7
Crystal size/mm^3	0.02 × 0.012 × 0.01

Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.52 to 54.18
Index ranges	$-13 \leq h \leq 14$, $-14 \leq k \leq 15$, $-16 \leq l \leq 16$
Reflections collected	24433
Independent reflections	6459 [R_{int} = 0.0513, R_{sigma} = 0.0600]
Data/restraints/parameters	6459/66/435
Goodness-of-fit on F^2	1.246
Final R indexes [I>=2σ (I)]	R_1 = 0.1043, wR_2 = 0.3178
Final R indexes [all data]	R_1 = 0.1414, wR_2 = 0.3471
Largest diff. peak/hole / e $Å^{-3}$	0.95/-1.11

Table S6. Bond Lengths Compound **4a**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N2	C8	1.437(4)	C9	C10	1.381(5)
N2	C7	1.396(4)	C20	C25	1.379(5)
N2	C14	1.354(4)	C20	C21	1.357(5)
N3	C18	1.357(4)	C6	C5	1.377(5)
N3	C15	1.374(4)	C27	C28	1.363(5)
N4	C19	1.358(4)	C30	C29	1.367(6)
N4	C26	1.384(4)	C13	C12	1.372(5)
N4	C20	1.446(4)	C5	C4	1.395(5)
N5	C19	1.356(4)	C25	C24	1.371(5)
N5	C31	1.389(4)	C3	C4	1.385(6)
N5	C32	1.448(5)	C28	C29	1.412(6)
N1	C14	1.354(4)	C10	C11	1.401(6)
N1	C2	1.394(4)	C11	C12	1.368(6)
N1	C1	1.476(5)	C24	C23	1.370(6)
C8	C9	1.379(5)	C23	C22	1.371(6)
C8	C13	1.378(4)	C21	C22	1.380(6)
C7	C2	1.388(5)	S1A	O2A	1.374(11)
C7	C6	1.380(5)	S1A	O1A	1.268(7)
C19	C18	1.441(5)	S1A	O3A	1.413(7)
C31	C26	1.390(5)	S1A	O4A	1.659(11)
C31	C30	1.393(5)	S1B	O2B	1.77(3)
C14	C15	1.436(5)	S1B	O1B	1.27(2)
C2	C3	1.382(5)	S1B	O3B	1.175(17)
C16	C17	1.379(5)	S1B	C33B	1.31(3)

C16	C15	1.399(5)	S1B	O4B	1.60(2)
C26	C27	1.400(5)	O2B	O3B	1.76(3)
C18	C17	1.416(4)	O1B	C33B	0.90(5)

Table S7. Bond Angles for Compound **4a**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	N2	C8	123.8(3)	C5	C6	C7	116.7(3)
C14	N2	C8	126.4(3)	C18	C17	C16	106.0(3)
C14	N2	C7	109.8(3)	C14	C15	N3	121.3(3)
C15	N3	C18	104.7(3)	C16	C15	N3	111.6(3)
C26	N4	C19	109.1(3)	C16	C15	C14	127.2(3)
C20	N4	C19	126.9(3)	C28	C27	C26	116.1(4)
C20	N4	C26	124.0(3)	C29	C30	C31	116.2(4)
C31	N5	C19	108.8(3)	C12	C13	C8	118.9(3)
C32	N5	C19	127.4(3)	C4	C5	C6	122.1(3)
C32	N5	C31	123.7(3)	C24	C25	C20	119.6(4)
C2	N1	C14	109.2(3)	C4	C3	C2	117.2(4)
C1	N1	C14	129.3(3)	C29	C28	C27	122.1(4)
C1	N1	C2	121.4(3)	C3	C4	C5	120.8(3)
C9	C8	N2	118.9(3)	C28	C29	C30	122.0(3)
C13	C8	N2	119.7(3)	C11	C10	C9	119.7(4)
C13	C8	C9	121.3(3)	C12	C11	C10	119.4(4)
C2	C7	N2	106.1(3)	C23	C24	C25	119.8(4)
C6	C7	N2	132.1(3)	C11	C12	C13	121.3(3)
C6	C7	C2	121.8(3)	C22	C23	C24	119.9(4)
N5	C19	N4	108.2(3)	C22	C21	C20	118.8(4)
C18	C19	N4	125.0(3)	C21	C22	C23	120.7(4)
C18	C19	N5	126.7(3)	O1A	S1A	O2A	106.5(6)
C26	C31	N5	107.1(3)	O3A	S1A	O2A	120.4(6)
C30	C31	N5	130.9(3)	O3A	S1A	O1A	123.0(5)
C30	C31	C26	121.9(3)	O4A	S1A	O2A	98.6(6)
N1	C14	N2	107.7(3)	O4A	S1A	O1A	110.8(7)
C15	C14	N2	124.6(3)	O4A	S1A	O3A	93.2(5)
C15	C14	N1	127.4(3)	O1B	S1B	O2B	105.2(15)
C7	C2	N1	107.2(3)	O3B	S1B	O2B	70.2(14)

C3	C2	N1	131.4(3)	O3B	S1B	O1B	137.8(15)
C3	C2	C7	121.4(3)	C33B	S1B	O2B	118(2)
C15	C16	C17	106.3(3)	C33B	S1B	O1B	41(2)
C31	C26	N4	106.8(3)	C33B	S1B	O3B	102(3)
C27	C26	N4	131.5(3)	O4B	S1B	O2B	89.9(13)
C27	C26	C31	121.6(3)	O4B	S1B	O1B	122.6(13)
C19	C18	N3	121.5(3)	O4B	S1B	O3B	99.5(13)
C17	C18	N3	111.4(3)	O4B	S1B	C33B	149(3)
C17	C18	C19	127.0(3)	O3B	O2B	S1B	38.8(8)
C10	C9	C8	119.2(3)	C33B	O1B	S1B	72(3)
C25	C20	N4	119.5(3)	O2B	O3B	S1B	71.0(14)
C21	C20	N4	119.4(3)	O1B	C33B	S1B	67(3)
C21	C20	C25	121.2(4)				

Table S8. Torsional angles for Compound **4a**

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
N2	C8	C9	C10	-179.1(3)	N5	C31	C26	C27	179.5(3)
N2	C8	C13	C12	178.4(3)	N5	C31	C30	C29	178.0(4)
N2	C7	C2	N1	-0.0(3)	N1	C14	C15	C16	148.7(3)
N2	C7	C2	C3	-178.7(3)	N1	C2	C7	C6	179.1(2)
N2	C7	C6	C5	178.1(4)	N1	C2	C3	C4	-178.3(4)
N2	C14	N1	C2	0.9(3)	C8	C9	C10	C11	1.2(4)
N2	C14	N1	C1	177.5(3)	C8	C13	C12	C11	0.0(4)
N2	C14	C15	N3	155.6(3)	C7	C2	C3	C4	0.1(4)
N2	C14	C15	C16	-26.0(4)	C7	C6	C5	C4	0.7(4)
N3	C18	C19	N4	-157.2(3)	C19	C18	C17	C16	177.7(4)
N3	C18	C19	N5	25.8(4)	C31	C26	C27	C28	2.8(4)
N3	C18	C17	C16	0.4(3)	C31	C30	C29	C28	0.9(4)
N3	C15	C14	N1	-29.7(4)	C14	C15	C16	C17	-179.1(4)
N3	C15	C16	C17	-0.6(3)	C2	C3	C4	C5	-0.1(4)
N4	C19	N5	C31	-1.7(3)	C26	C27	C28	C29	-1.0(4)
N4	C19	N5	C32	-178.9(3)	C9	C10	C11	C12	-1.7(4)
N4	C19	C18	C17	25.8(4)	C20	C25	C24	C23	0.7(5)
N4	C26	C31	N5	-0.9(3)	C20	C21	C22	C23	0.0(6)
N4	C26	C31	C30	176.9(3)	C6	C5	C4	C3	-0.3(4)
N4	C26	C27	C28	-176.8(4)	C27	C28	C29	C30	-0.8(4)

N4	C20	C25	C24	177.5(3)	C13	C12	C11	C10	1.1(5)
N4	C20	C21	C22	-177.9(4)	C25	C24	C23	C22	0.1(5)
N5	C19	C18	C17	-151.2(3)	C24	C23	C22	C21	-0.4(6)

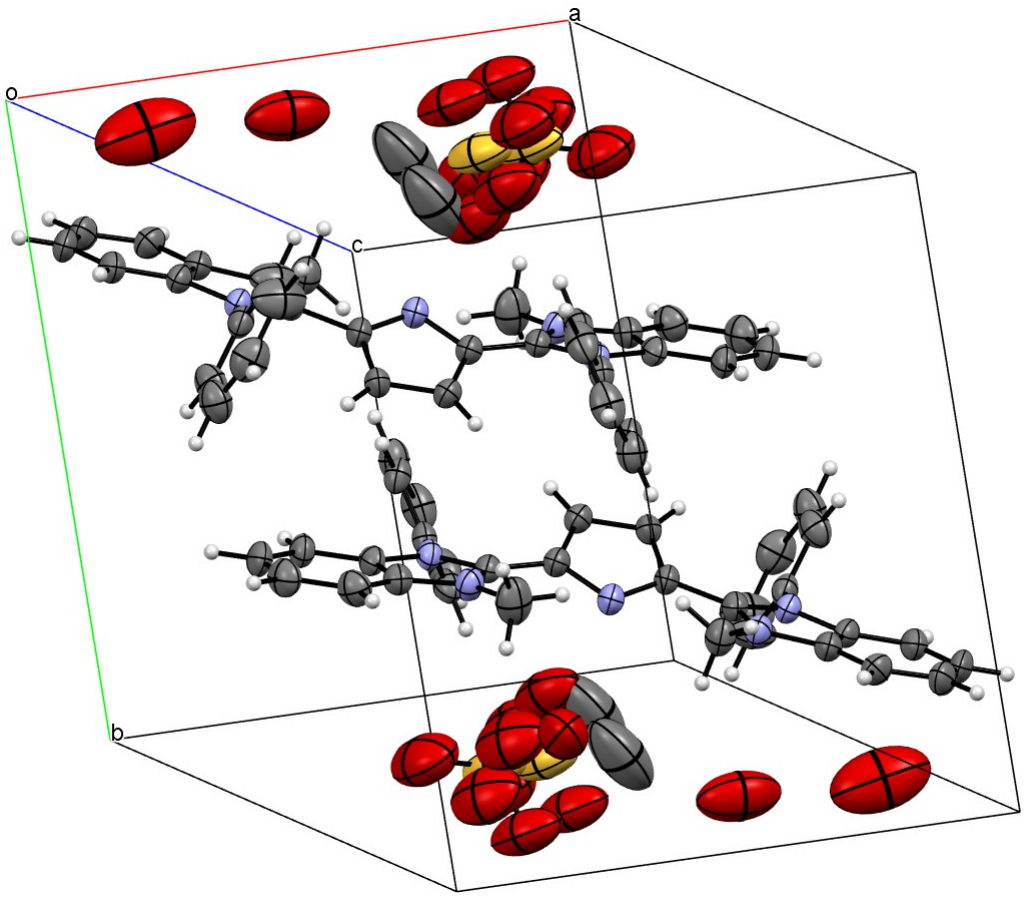


Figure S34. Crystal packing of Compound **4a** in unit cell

CheckCIF report of compound 4a crystal structure

Datablock: ex-nipphe_autored

Bond precision: C-C = 0.0057 A Wavelength=0.71073

Cell: a=11.0277(5) b=12.5158(4) c=13.0402(5)
alpha=72.121(4) beta=65.597(4) gamma=88.754(3)

Temperature: 222 K

	Calculated	Reported
Volume	1548.36(13)	1548.36(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H26 N5, 0.3(C O4 S), 0.7(O4 S), 3(O), 0.7(C)	C32 H26 N5, 0.3(C O4 S), 0.7(O4 S), 3(O), 0.7(C)
Sum formula	C33 H26 N5 O7 S	C33 H26 N5 O7 S
Mr	636.65	636.65
Dx,g cm-3	1.366	1.366
Z	2	2
Mu (mm-1)	0.162	0.162
F000	662.0	662.7
F000'	662.56	
h,k,lmax	14,16,16	14,15,16
Nref	6824	6459
Tmin,Tmax	0.998,0.998	
Tmin'	0.997	

Correction method= Not given

Data completeness= 0.947 Theta(max)= 27.090

R(reflections)= 0.1043(4074) wR2(reflections)= 0.3471(6459)

S = 1.246 Npar= 435

.

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O5 Check

Author Response: Hydrogen atoms of the solvent water were not located hence refined with

And 2 other PLAT306 Alerts
More ...
PLAT430_ALERT_2_B Short Inter D...A Contact O4A ..O5 . 2.74 Ang.
x,y,z = 1_555 Check

Author Response: Disordered in the Oxygen atoms of the CH3O4S ion

PLAT430_ALERT_2_B Short Inter D...A Contact O5 ..O5 . 2.71 Ang.
1-x,-y,1-z = 2_656 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O5 ..N3 . 2.84 Ang.
1-x,-y,1-z = 2_656 Check
And 2 other PLAT430 Alerts
More ...
1-x,-y,-z = 2_655 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O7 ..O7 . 2.67 Ang.
1-x,-y,-z = 2_655 Check

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.35 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1B 0.160 Check
And 5 other PLAT260 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00572 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact O3A ..O6 . 2.89 Ang.
x,y,z = 1_555 Check

Author Response: Disordered in the Oxygen atoms of the CH3O4S ion

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.967 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note
1 0 0, -1 1 0, 0 1 0, 1 1 0, 0 -1 1, 1 -1 1,
0 0 1, 1 0 1, 0 1 1, 1 1 1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
2 0 0, -2 -1 1, -2 0 1, 3 0 1, -1 1 1, -1 2 1,
5 13 9,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.68Ang From O5 . -0.48 eA-3
And 2 other PLAT976 Alerts
More ...

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 12 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT073_ALERT_1_G H-atoms ref, but _hydrogen_treatment Reported as constr Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0030 Report
And 3 other PLAT190 Alerts
More ...
PLAT300_ALERT_4_G Atom Site Occupancy of S1B Constrained at 0.3 Check
And 11 other PLAT300 Alerts
More ...
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
And 2 other PLAT302 Alerts
More ...
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2) 1.80 Check
And 2 other PLAT304 Alerts
More ...
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1B . 71.8 Degree
And 2 other PLAT395 Alerts
More ...
PLAT432_ALERT_2_G Short Inter X...Y Contact O5 ..C33A . 2.76 Ang.
x,y,z = 1_555 Check

And 2 other PLAT432 Alerts

More ...

1-x,-y,1-z = 2_656 Check

PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data Please Note

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 41.00 Deg.
C33B -S1B -O1B 1_555 1_555 1_555 ..... # 126 Check

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.80 Deg.
O3B -O2B -S1B 1_555 1_555 1_555 ..... # 132 Check

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 66 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 342 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
-2 -1 1, -2 0 1, -1 1 1, -1 2 1, 2 0 0, 3 0 1,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 5.592 Note
Predicted wR2: Based on SigI**2 6.21 or SHELX Weight 27.86

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

PLAT983_ALERT_1_G The S-f"= 0.1245 Deviates from IT-Value = 0.1234 Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
9 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
45 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
31 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
26 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Ellipsoid plot from CheckCIF report of compound 4a crystal structure

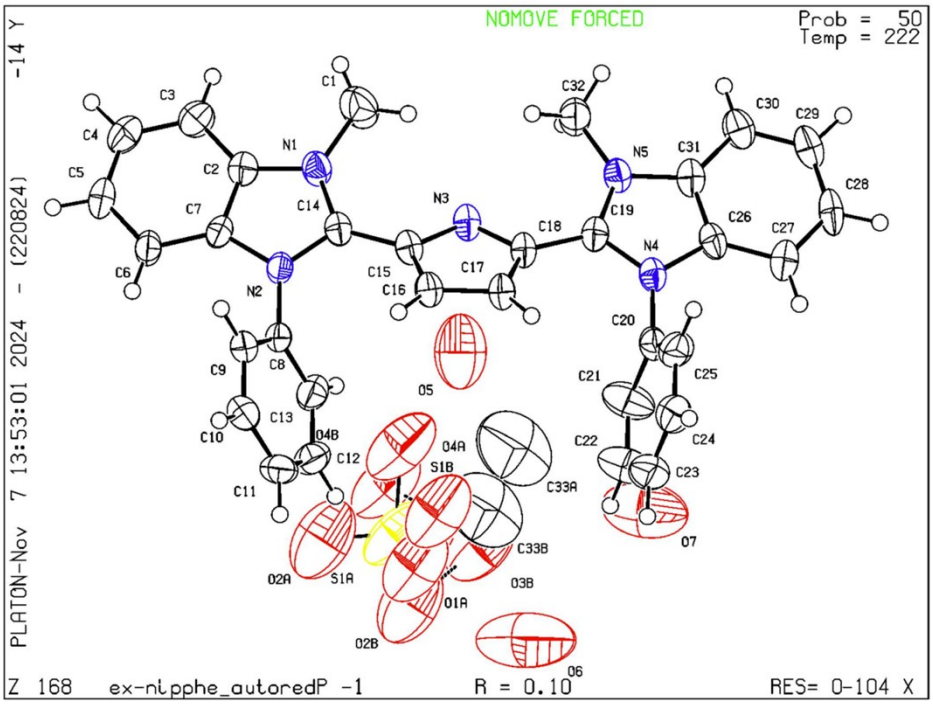


Table S9. The comparison of geometric parameters from SCXRD with optimization done using M06-2X/def2tzvpp and B3LYP/6-31+G(d) level of theory.

Geometric Parameters		M06-2X/def2tzvpp	B3LYP/6-31+G(d)	X-Ray Structure
Bond Lengths (Å)	N3-C15	1.348	1.361	1.375
	N3-C18	1.348	1.361	1.358
	C-15-C16	1.418	1.428	1.399
	C-17-C18	1.418	1.428	1.417
	C-18-C19	1.434	1.439	1.441
	C14-C15	1.434	1.439	1.433
Bond Angles (°)	C18-N3-C15	104.96	105.25	104.70
	C19-C18-N3	119.92	120.56	121.52
	C14-C15-N3	119.92	120.56	121.25
	C17-C18-N3	111.91	111.51	111.38
	C16-C15-N3	111.91	111.51	111.60
Dihedral angles (°)	N5-C19-C18-N3	-21.92	-23.96	25.64
	N1-C14-C15-N3	-21.92	-23.95	-29.63
	N5-C19-C18-C17	157.45	154.62	-151.22
	N1-C14-C15-C16	157.45	154.62	148.66

Computational details

Density functional theory (DFT) calculations were carried out using Gaussian16 suite of programs.[19] All the geometry optimizations were performed by using the M06-2X/def2tzvpp level of theory. Au atom was modelled using LANL2DZ basis set using effective core potentials. Sum of electronic and zero-point energies were used for calculating the singlet-triplet energy gap. All the minima are characterized by zero negative frequencies. NICS (in ppm) and NMR calculations was calculated at the GIAO/M06-2X/def2tzvpp level of theory while the anisotropy of the induced current density (ACID) was calculated at the CGST/M06-2X/def2tzvpp level of theory for all the compounds. The proton affinity values are obtained using equation 1.

$$D + H^+ \rightarrow DH^+$$

$$PA = -(E_{DH^+} - E_D - 0.01) \quad \text{..... Equation 1}$$

Where E_D and E_{DH^+} are the enthalpy values of a parent compound and protonated compound, respectively.

The gas phase hydride ion affinity at 298.15 K was obtained using equation 2.

$$X + H^- \rightarrow XH^-$$

$$HIA = -(E_{XH} - E_{X^+} - E_{H^-}) \quad \text{..... Equation 2}$$

Where E_{X+} and E_{XH} are the energy values of a parent compound and its complex with hydride ion, respectively.

Complexation energies with Lewis acids like BH_3 and AuCl was calculated using equation 3 and 4.

$$\Delta E_{BH3} = E_{complex} - (E_{Mol} + E_{BH3}) \quad \text{..... Equation 3}$$

$$\Delta E_{AuCl} = E_{complex} - (E_{Mol} + E_{AuCl}) \quad \text{..... Equation 4}$$

Where ΔE is the energy of complexation and E_{Mol} is the absolute Gibbs free energy of a given molecule.

Energy Decomposition Analysis (EDA)[20-24] is a state-of-the-art electronic structure method that is being used to understand and study the nature of chemical bonds throughout the

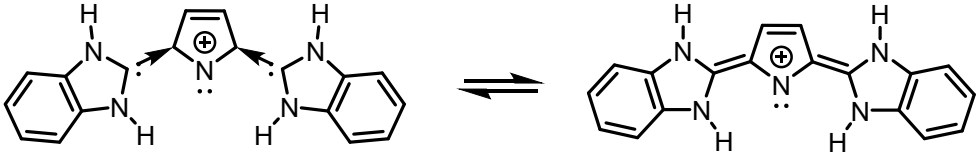
periodic table. Originally reported and developed by Kitaura and Morokuma[25] and by Ziegler and Rauk[26] independently, EDA calculates the ΔE_{int} (instantaneous interaction energy) using equation 1. All these energies are calculated between the defined fragments in the keeping them in the geometry as in the molecule.

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{pauli} + \Delta E_{orb} \quad \text{.....eq. 1}$$

ΔE_{elstat} is an attractive term that comes because of the electrostatic (coulombic) interactions between the unperturbed charge densities of the fragments in their frozen geometry of the molecule. ΔE_{Pauli} is a repulsive term that calculates the increase in the energy because of repulsive interactions due to the electrons with the same spin. ΔE_{orb} is the stabilizing energy that comes from the overlap of orbitals of fragments in frozen geometry of the molecule. ΔE_{orb} can be decomposed into various contributions from the different natural orbitals for chemical valance and can be studied using EDA-NOCV developed by Mitoraj and Michalak.[27-31] All EDA calculations were performed at BP86/TZ2P level of theory using ADF-2020.102 program package.[32, 33]

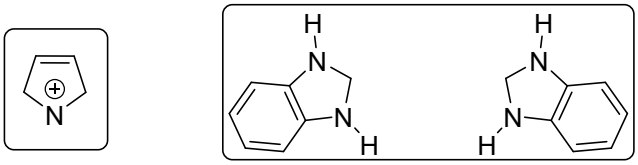
To perform the EDA analysis, a model compound **4g** was prepared by substituting the nitrogen centres at benzimidazole rings with hydrogen atoms. The compound was optimized in c2v symmetry to overcome the convergence problems. Please note that the molecule remains planar (as in c2v symmetry) even if no symmetry constraints were enforced for optimization. Also, the structure optimized in c2v symmetry and the structure optimized without any symmetry constraints are same in energy. In compound **4a** and **4b,** it is because of the sterics imposed by the -Me or -Ph substituents at the benzimidazole ring, that we see a twist or change in the dihedral between two benzimidazole rings. The optimization of compound **4g** was performed at M062X/def2TZVPP level.

Scheme S8. Donor-Acceptor and Electron sharing bonding situations considered in this work.



4g$_1$ **4g$_2$**

Scheme S9. Fragmentation of compound model compound **4g** for EDA analysis.



F1 **F2**

Table S10. EDA-NOCV results of the best possible bonding representation of model compound **4g** at the BP86/TZ2P level of theory. Energies are in kcal/mol. The corresponding deformation density plots are given in Scheme S8.

	4g$_1$	**4g$_2$**
ΔE_{int}	-365.37	-500.89
ΔE_{pauli}	717.77	517.76
ΔE_{elstat}	-425.07	-321.81
ΔE_{orb}	-658.07	-696.85

Values in italics give the percentage contribution to the total interaction energy.

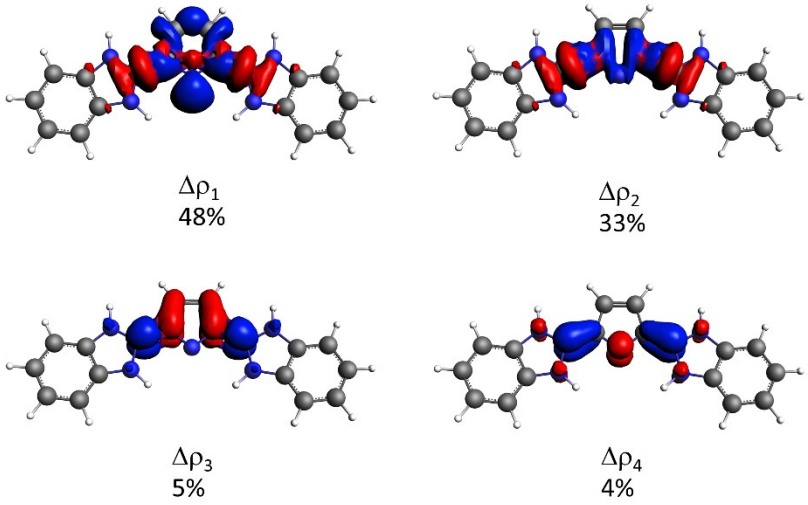
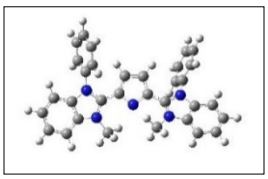


Figure S35. The plots for deformation densities for **4g$_1$** along-with their percentage contribution to the total orbital interaction energy (isosurface value = 0.001).

List of Coordinates of all the optimized geometries at m06-2x/def2tzvpp level of theory

Compound 4a (Singlet)

Absolute Energy = -1508.149868 a.u.

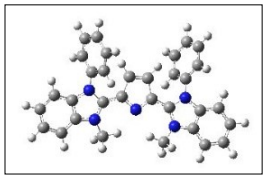


1 1

C	1.06385500	0.02034200	-0.11053000
C	0.68505700	-1.34583800	-0.06436100
C	-0.68506800	-1.34583600	0.06437700
C	-1.06386300	0.02034400	0.11055000
C	-2.37996800	0.57049600	0.26515300
C	-4.60719500	0.78337500	0.26521100
C	-4.05423200	1.97434900	0.72379800
N	-2.67489500	1.80303100	0.72192400
N	-3.54105300	-0.06436300	-0.01480400
C	-1.74024500	2.79793000	1.22469600
H	-0.91837300	2.29895600	1.72485300
H	-1.34301300	3.39427100	0.40631900
H	-2.27717600	3.43318700	1.92363600
C	2.37995800	0.57049800	-0.26513600
C	4.05420500	1.97436700	-0.72380000
C	4.60718300	0.78339500	-0.26522700
N	3.54105200	-0.06435200	0.01480500
N	2.67486900	1.80303900	-0.72190100
C	1.74019500	2.79793200	-1.22464200
H	1.34292700	3.39421900	-0.40624400
H	2.27711800	3.43324000	-1.92354300
H	0.91834900	2.29895600	-1.72483900
N	-0.00000500	0.84164800	-0.00000500
H	1.32489100	-2.20916000	-0.13063100
H	-1.32490600	-2.20915600	0.13064900
C	5.97629700	0.60778100	-0.13449500
C	4.85314400	3.05196000	-1.08090100
C	6.22122700	2.87955100	-0.95982100
C	6.77326100	1.68058100	-0.49334100
H	6.39253700	-0.31959400	0.23244300
H	7.84692800	1.59264600	-0.40885200
H	6.87979800	3.69346500	-1.22728200
H	4.43558700	3.98547500	-1.42894200
C	-4.85318400	3.05193700	1.08089000
C	-5.97630600	0.60775400	0.13445500
C	-6.77328300	1.68054800	0.49329300
C	-6.22126300	2.87952000	0.95978600
H	-4.43563700	3.98545200	1.42894200
H	-6.87984500	3.69342800	1.22723900
H	-7.84694700	1.59260700	0.40878500
H	-6.39253400	-0.31962200	-0.23249200
C	-3.69742200	-1.36376800	-0.59659800
C	-3.31660100	-1.57309100	-1.91258100
C	-4.25060100	-2.37780000	0.16902300
C	-3.47733900	-2.83404100	-2.46516700
H	-2.88955400	-0.76049800	-2.48445600
C	-4.41479400	-3.63463400	-0.39601400
H	-4.53806800	-2.18207900	1.19368300
C	-4.02425400	-3.86268500	-1.70842000
H	-3.17954500	-3.01206900	-3.48886000
H	-4.84335700	-4.43453100	0.19126600
H	-4.15034200	-4.84373400	-2.14479000
C	3.69744400	-1.36375300	0.59660000
C	4.25060400	-2.37778600	-0.16903300
C	3.31666600	-1.57307200	1.91259600
C	4.41482000	-3.63461700	0.39600400
H	4.53803900	-2.18206900	-1.19370400
C	3.47742600	-2.83401900	2.46518300
H	2.88963300	-0.76047800	2.48448100
C	4.02432100	-3.86266400	1.70842300
H	4.84336800	-4.43451500	-0.19128600
H	3.17966500	-3.01204400	3.48888500
H	4.15042600	-4.84371100	2.14479300

Compound 4a (Triplet)

Absolute Energy = -1508.055979 a.u.



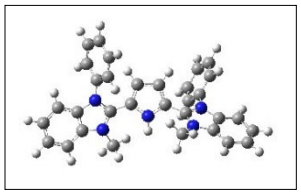
1 3

C	-1.08443900	0.17256600	0.05980900
C	-0.66763600	-1.24533600	0.03003400
C	0.66763800	-1.24533700	-0.02998600
C	1.08444100	0.17256300	-0.05978300
C	2.39353300	0.65070700	-0.18050700
C	4.64608500	0.70297200	-0.27582000
C	4.15750200	1.97665300	-0.58803500
N	2.78617700	1.92856700	-0.51243800
N	3.54987200	-0.09708100	-0.02702900
C	1.96331200	3.06044400	-0.90546700
H	0.92202900	2.76805700	-0.88411600
H	2.13350600	3.88532400	-0.21321400
H	2.24974600	3.37332900	-1.90950200

C	-2.39353500	0.65070900	0.18052100
C	-4.15751900	1.97664200	0.58803200
C	-4.64608900	0.70295500	0.27581900
N	-3.54986800	-0.09708600	0.02703100
N	-2.78619300	1.92856900	0.51244400
C	-1.96334900	3.06045800	0.90548000
H	-2.13354300	3.88533300	0.21322100
H	-2.24980400	3.37334500	1.90950800
H	-0.92206200	2.76808800	0.88414800
N	0.00000200	0.99486400	0.00000900
H	-1.30988900	-2.10755100	0.07286600
H	1.30989100	-2.10755300	-0.07280500
C	-6.00793400	0.43763700	0.22576500
C	-5.01309900	3.02650200	0.89904800
C	-6.37074000	2.75651900	0.86629400
C	-6.85855900	1.48723300	0.52961400
H	-6.38124300	-0.54102100	-0.03905300
H	-7.92649000	1.32378000	0.50607500
H	-7.07199400	3.54480300	1.09987900
H	-4.63773100	4.00880200	1.14708600
C	5.01307100	3.02652100	-0.89905800
C	6.00793200	0.43766600	-0.22577200
C	6.85854700	1.48726900	-0.52962900
C	6.37071500	2.75654900	-0.86631000
H	4.63769300	4.00881600	-1.14709600
H	7.07196000	3.54483900	-1.09990100
H	7.92647900	1.32382600	-0.50609600
H	6.38125200	-0.54098800	0.03904500
C	3.65202300	-1.39512700	0.55561700
C	3.21656700	-1.59989100	1.85797700
C	4.20770700	-2.42616200	-0.18733200
C	3.32358300	-2.86455700	2.41450100
H	2.79536400	-0.77552400	2.41820900
C	4.31954500	-3.68668200	0.38259100
H	4.53553500	-2.23913200	-1.20141700
C	3.87350800	-3.90705300	1.67859900
H	2.98469700	-3.03430900	3.42689200
H	4.74933600	-4.49682900	-0.18972000
H	3.95840800	-4.89106000	2.11808800
C	-3.65200700	-1.39513100	-0.55562100
C	-4.20767700	-2.42617600	0.18732500
C	-3.21655800	-1.59988200	-1.85798600
C	-4.31950600	-3.68669300	-0.38260400
H	-4.53550100	-2.23915400	1.20141300
C	-3.32356400	-2.86454700	-2.41451600
H	-2.79536700	-0.77550900	-2.41821600
C	-3.87347400	-3.90705200	-1.67861700
H	-4.74928500	-4.49684700	0.18970500
H	-2.98468400	-3.03428900	-3.42691100
H	-3.95836800	-4.89105800	-2.11811000

Compound 4a (Protonated)

Absolute Energy = -1508.435890 a.u.



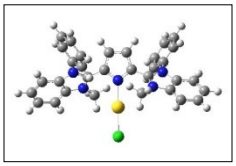
2 1

C	-1.10078400	-0.02730600	0.18474300
C	-0.69290800	-1.34425300	0.10889400
C	0.69288300	-1.34426300	-0.10906000
C	1.10078700	-0.02732100	-0.18484800
C	2.43316800	0.49952400	-0.41086900
C	4.64486900	0.70048800	-0.35646800
C	4.13421000	1.72295100	-1.14995800
N	2.75366400	1.55942100	-1.16944200
N	3.55444800	-0.03783900	0.09102400
C	1.86037700	2.35311800	-2.00206900
H	0.96726300	1.77762200	-2.22749400
H	1.60298600	3.28901100	-1.50739200
H	2.37243500	2.57640000	-2.93457900
C	-2.43315000	0.49954900	0.41082600
C	-4.13416600	1.72298700	1.14996000
C	-4.64485300	0.70052100	0.35649300
N	-3.55444900	-0.03782100	-0.09101700
N	-2.75362000	1.55944300	1.16941600
C	-1.86031300	2.35313300	2.00202700
H	-1.60291800	3.28902100	1.50734200
H	-2.37235700	2.57642800	2.93454200
H	-0.96720400	1.77762800	2.22744800
N	-0.00000400	0.76902800	-0.00011500
H	-1.33022200	-2.20660400	0.20621000
H	1.33018500	-2.20662300	-0.20637800
C	-6.00719800	0.56167200	0.11658900
C	-4.96023000	2.66274100	1.75772100
C	-6.31363500	2.52318300	1.52657300
C	-6.82739200	1.49319600	0.71895000
H	-6.39492000	-0.23013600	-0.50826300
H	-7.89547500	1.43281900	0.56615400
H	-6.99966400	3.22715100	1.97560600
H	-4.57229100	3.46302700	2.37149800
C	4.96029700	2.66269200	-1.75770700
C	6.00720700	0.56163100	-0.11652800
C	6.82742300	1.49314300	-0.71887700
C	6.31369500	2.52312700	-1.52652200
H	4.57238000	3.46297700	-2.37149900
H	6.99974000	3.22708600	-1.97554200
H	7.89550200	1.43276200	-0.56605000
H	6.39490700	-0.23017200	0.50834300
C	3.65546300	-1.17555800	0.96794000
C	3.21685400	-1.06840500	2.27762500

C	4.22115200	-2.34121300	0.47515800
C	3.33277100	-2.17077000	3.11121800
H	2.80455800	-0.13544500	2.63864300
C	4.33658700	-3.43514600	1.32116600
H	4.56417700	-2.38845000	-0.55041300
C	3.88959300	-3.35026700	2.63337300
H	3.00120500	-2.10396900	4.13776700
H	4.77760500	-4.35126300	0.95447700
H	3.98480200	-4.20401500	3.28957400
C	-3.65549200	-1.17555300	-0.96791200
C	-4.22117100	-2.34120000	-0.47509800
C	-3.21691700	-1.06842000	-2.27761000
C	-4.33663500	-3.43514300	-1.32108800
H	-4.56416900	-2.38842000	0.55048300
C	-3.33286300	-2.17079600	-3.11118500
H	-2.80462700	-0.13546700	-2.63865200
C	-3.88967700	-3.35028400	-2.63331000
H	-4.77764800	-4.35125300	-0.95437500
H	-3.00132500	-2.10401000	-4.13774500
H	-3.98490900	-4.20404000	-3.28949700
H	-0.00000100	1.77573900	-0.00014300

Compound 4a complex with AuCl

Absolute Energy = -2103.744950 a.u.

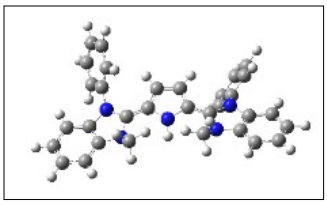


1 1

C	1.04958100	1.10992600	0.26647200
C	0.67846400	2.44833700	0.16068200
C	-0.67858900	2.44831600	-0.16061800
C	-1.04965100	1.10989400	-0.26649400
C	-2.36477400	0.58246100	-0.58318600
C	-4.56413700	0.24001200	-0.50142300
C	-4.03844400	-0.50953300	-1.54913400
N	-2.67404300	-0.26079400	-1.57548900
N	-3.48949700	0.90554300	0.07986900
C	-1.78152600	-0.77536700	-2.60448100
H	-0.83209200	-0.25365100	-2.53786200
H	-1.62183300	-1.84257600	-2.45676900
H	-2.23821400	-0.59354000	-3.57548300
C	2.36471800	0.58251300	0.58315000
C	4.03836700	-0.50957800	1.54901800
C	4.56407200	0.24003000	0.50135800
N	3.48944500	0.90563400	-0.07987700
N	2.67397200	-0.26081000	1.57539400
C	1.78143100	-0.77545800	2.60432500
H	1.62179100	-1.84266300	2.45653200
H	2.23805500	-0.59366800	3.57536500
H	0.83197600	-0.25378300	2.53768600
N	-0.00002000	0.29163200	-0.00001800
H	1.31795100	3.30282300	0.30697900
H	-1.31811500	3.30278200	-0.30685900
C	5.91591900	0.20935200	0.18356100
C	4.83848900	-1.32066500	2.34439500
C	6.18472100	-1.34488000	2.03707400
C	6.71272400	-0.59600700	0.97388500
H	6.31613400	0.77931500	-0.64248100
H	7.77133800	-0.65644100	0.76552600
H	6.84874300	-1.96284700	2.62428200
H	4.42893300	-1.91103800	3.15141800
C	-4.83858500	-1.32054300	-2.34457100
C	-5.91598600	0.20934600	-0.18363500
C	-6.71280900	-0.59593700	-0.97401800
C	-6.18482000	-1.34474700	-2.03725800
H	-4.42904200	-1.91087300	-3.15163200
H	-6.84885500	-1.96265700	-2.62451300
H	-7.77142500	-0.65636100	-0.76566600
H	-6.31618900	0.77926100	0.64244700
C	-3.56797100	1.71175500	1.26255200
C	-2.87757500	1.31829000	2.39848700
C	-4.35387500	2.85249700	1.24580400
C	-2.97147200	2.09715900	3.54078400
H	-2.28320200	0.41379000	2.37840300
C	-4.44670200	3.61968600	2.39837200
H	-4.87748800	3.13522200	0.34189700
C	-3.75469900	3.24445300	3.54133000
H	-2.44137700	1.80216600	4.43542100
H	-5.05650100	4.51210900	2.39970800
H	-3.82908300	3.84510400	4.43701800
C	3.56792800	1.71192200	-1.26250700
C	4.35385700	2.85264600	-1.24568700
C	2.87752100	1.31854400	-2.39846500
C	4.44670000	3.61990700	-2.39820800
H	4.87747800	3.13530100	-0.34176400
C	2.97143500	2.09748400	-3.54071300
H	2.28313100	0.41405400	-2.37843700
C	3.75468800	3.24476100	-3.54118800
H	5.05652000	4.51231500	-2.39948800
H	2.44133300	1.80256000	-4.43536800
H	3.82908500	3.84546700	-4.43683800
Au	0.00006800	-1.79370300	0.00003600
Cl	0.00015000	-4.06867700	0.00002900

Compound 4a + Hydride ion

Absolute Energy = -1508.859776 a.u.

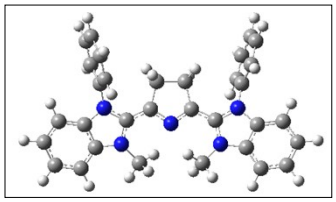


0 1

C	-1.19095400	-0.12607000	-0.32652900
C	-0.70000000	1.22006400	-0.47921900
C	0.65067300	1.21270800	-0.46604500
C	1.11666800	-0.14305800	-0.28090500
C	2.36000100	-0.64463300	-0.10419000
C	4.53469200	-0.79673700	0.57079000
C	3.97163800	-2.07815900	0.60709300
N	2.64517000	-2.00144800	0.18110000
N	3.55608300	0.08012500	0.10289700
C	2.13011600	-3.08279600	-0.64545300
H	1.99192400	-3.97846300	-0.04081900
H	1.17487500	-2.78852500	-1.06690200
H	2.82507800	-3.31176900	-1.45915100
C	-2.46852200	-0.58046700	-0.28563600
C	-4.29453000	-1.93216600	-0.30208000
C	-4.74607300	-0.62202300	-0.11918600
N	-3.62202400	0.20493900	-0.10692500
N	-2.90431200	-1.91151200	-0.36384900
C	-2.21965100	-2.94242600	-1.11827600
H	-2.40312900	-3.91153300	-0.65583900
H	-2.58366800	-2.97019600	-2.14944300
H	-1.15467600	-2.74368300	-1.12724500
N	-0.04313100	-0.98263300	-0.25416200
H	-1.31855700	2.09012300	-0.62449300
H	1.27984000	2.07766200	-0.58165600
C	-6.08719400	-0.34167800	0.03253000
C	-5.17779500	-2.98578900	-0.40531500
C	-6.54151400	-2.70486700	-0.27127900
C	-6.98379700	-1.41280700	-0.04427700
H	-6.43418200	0.66760000	0.20154200
H	-8.04179800	-1.22131000	0.06825700
H	-7.25718500	-3.51180100	-0.34353300
H	-4.83077200	-3.99586300	-0.57242300
C	4.72418900	-3.17985900	0.95268900
C	5.86131300	-0.59432100	0.89400200
C	6.61736000	-1.70860700	1.27066700
C	6.06322300	-2.97660100	1.30051800
H	4.29312800	-4.17157800	0.95265100
H	6.67119200	-3.82289400	1.58804600
H	7.65708000	-1.57213000	1.53395700
H	6.31021500	0.38651100	0.83736600
C	3.84821600	1.35130300	-0.43198200
C	3.53344900	1.64887300	-1.75652100
C	4.47517600	2.30749900	0.36109800
C	3.84135900	2.89468100	-2.27567100
H	3.03308900	0.90208300	-2.35890600
C	4.79353400	3.54865500	-0.17152000
H	4.69193100	2.07581900	1.39516400
C	4.47597300	3.84860100	-1.48823200
H	3.59106100	3.12025600	-3.30357000
H	5.27940800	4.28744400	0.45150000
H	4.71704800	4.81938400	-1.89867200
C	-3.65205600	1.50837800	0.44721700
C	-4.40527600	2.49375500	-0.17866400
C	-2.96020700	1.79780500	1.61971900
C	-4.47324200	3.76675900	0.37162400
H	-4.92292900	2.25641400	-1.09863500
C	-3.02061900	3.07348900	2.15432700
H	-2.36731700	1.02493900	2.08933600
C	-3.77829700	4.06103400	1.53497300
H	-5.06116500	4.53070500	-0.11880700
H	-2.47759800	3.29732600	3.06246400
H	-3.82311200	5.05520500	1.95782700
H	-0.04938400	-1.60126100	0.55094800

Compound 4a (ASE)

Absolute Energy = -1509.310344 a.u.



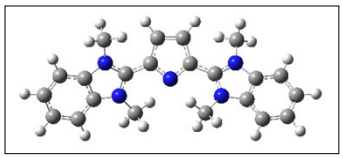
1 1

C	-1.09024700	0.00631600	-0.04585700
C	-0.75922000	1.47854400	0.12785200
C	0.75925200	1.47854400	-0.12787300
C	1.09026800	0.00632000	0.04585900
C	2.36535200	-0.57520800	0.19510400
C	4.59981600	-0.81398100	0.30348900
C	4.01530500	-2.02931000	0.64879900
N	2.63873200	-1.85014400	0.58323800
N	3.55827900	0.06582800	0.02650300
C	1.67663600	-2.85651500	0.98746500
H	0.91388300	-2.40353200	1.61378800
H	1.19657500	-3.30479800	0.11976300
H	2.20780900	-3.61923900	1.54907000
C	-2.36533600	-0.57521300	-0.19510200
C	-4.01530000	-2.02931300	-0.64879100
C	-4.59980600	-0.81397800	-0.30350400
N	-3.55826700	0.06582400	-0.02650700
N	-2.63872600	-1.85015000	-0.58323600
C	-1.67664800	-2.85653700	-0.98746200

H	-1.19655400	-3.30478400	-0.11976200
H	-2.20784900	-3.61928200	-1.54901300
H	-0.91391900	-2.40358500	-1.61383800
N	0.00001100	-0.75390400	0.00000700
H	-1.30176500	2.13573100	-0.54766300
H	1.30180300	2.13574000	0.54762800
C	-5.97292800	-0.64415000	-0.25501300
C	-4.79067300	-3.13241400	-0.97245500
C	-6.16700700	-2.96542100	-0.93670200
C	-6.74834600	-1.74581700	-0.58241100
H	-6.41286500	0.30166100	0.02784500
H	-7.82521400	-1.66002500	-0.55913700
H	-6.80429500	-3.80261100	-1.18304800
H	-4.35368700	-4.08531600	-1.23288700
C	4.79067400	-3.13241300	0.97246500
C	5.97293900	-0.64416500	0.25497900
C	6.74835200	-1.74583400	0.58238300
C	6.16700800	-2.96543000	0.93669300
H	4.35368600	-4.08531300	1.23290200
H	6.80429400	-3.80262200	1.18303800
H	7.82522100	-1.66004900	0.55909700
H	6.41288100	0.30164000	-0.02789200
C	3.77285100	1.37000700	-0.51916300
C	3.52758800	1.59668600	-1.86491500
C	4.27489600	2.37107100	0.29904000
C	3.76247100	2.85769500	-2.39265000
H	3.15459400	0.79076300	-2.48360000
C	4.51471200	3.62720900	-0.23858100
H	4.46713600	2.16244400	1.34333100
C	4.25389200	3.87127000	-1.58057200
H	3.57048200	3.04547500	-3.43981800
H	4.90295500	4.41510300	0.39155300
H	4.44066400	4.85174600	-1.99599400
C	-3.77285000	1.36999800	0.51916800
C	-4.27484900	2.37107800	-0.29904300
C	-3.52766200	1.59665000	1.86493800
C	-4.51467800	3.62721000	0.23858600
H	-4.46703900	2.16246900	-1.34334700
C	-3.76256000	2.85765200	2.39268200
H	-3.15470800	0.79071200	2.48362900
C	-4.25392400	3.87124600	1.58059400
H	-4.90288100	4.41511900	-0.39155500
H	-3.57062500	3.04541200	3.43986400
H	-4.44070800	4.85171800	1.99602200
H	0.97996400	1.80621400	-1.14576900
H	-0.97993000	1.80623500	1.14574000

Compound 4b (Singlet)

Absolute Energy = **-**1124.779583 a.u.



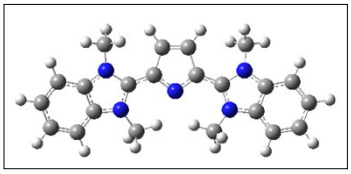
1 1

C	-1.06872300	0.98860600	-0.00577000
C	-0.69008900	2.35185200	0.00164700
C	0.68995400	2.35187800	-0.00084900
C	1.06866600	0.98865900	0.00612300
C	2.39775700	0.44202600	0.04049000
C	4.59437200	0.19793000	-0.24503900
C	4.11344400	-0.92456300	0.42343200
N	2.74968100	-0.73276600	0.59467300
N	3.50012400	1.01877400	-0.47814800
C	1.88950600	-1.64475300	1.33280900
H	1.09564300	-1.08080500	1.80829200
H	1.44760400	-2.37755500	0.66138200
H	2.49784100	-2.14365000	2.08264700
C	-2.39778100	0.44194100	-0.04032700
C	-4.11332900	-0.92482500	-0.42326800
C	-4.59445700	0.19788700	0.24469300
N	-3.50031100	1.01887700	0.47776400
N	-2.74951200	-0.73305400	-0.59419800
C	-1.88900400	-1.64514500	-1.33185300
H	-1.44549300	-2.37638800	-0.65980800
H	-2.49754000	-2.14584900	-2.08030600
H	-1.09631200	-1.08098100	-1.80905600
N	-0.00001000	0.16680600	0.00004600
H	-1.33215100	3.21599000	-0.02374400
H	1.33200100	3.21602500	0.02484000
C	-5.93769200	0.33884800	0.56376500
C	-4.95346700	-1.96468600	-0.79694600
C	-6.29277000	-1.82733000	-0.47805600
C	-6.77646800	-0.69597000	0.18992000
H	-6.31684500	1.21402800	1.07144500
H	-7.83071100	-0.62888600	0.41718200
H	-6.98296200	-2.61280000	-0.75061700
H	-4.58489400	-2.84323000	-1.30628600
C	4.95364700	-1.96434700	0.79714300
C	5.93748700	0.33872100	-0.56466500
C	6.77635300	-0.69601700	-0.19076700
C	6.29285300	-1.82713900	0.47774500
H	4.58519700	-2.84270600	1.30689700
H	6.98310800	-2.61255000	0.75031700
H	7.83051500	-0.62905300	-0.41843800
H	6.31649900	1.21371200	-1.07277600
C	3.55826100	2.24475700	-1.25558100
C	-3.55856500	2.24493200	1.25511300
H	-2.61253500	2.38840400	1.76830300
H	-3.76431200	3.10083100	0.61445900
H	-4.35392000	2.14338400	1.98882400

H	4.35298900	2.14287500	-1.98993100
H	2.61189100	2.38859100	-1.76803100
H	3.76485800	3.10057800	-0.61509700

Compound 4b (Triplet)

Absolute Energy = -1124.679427 a.u.

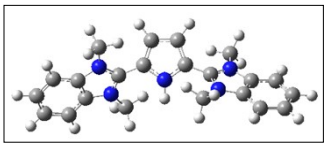


1 3

C	-1.08845500	0.89250800	0.02563600
C	-0.66785800	2.30852100	0.02325500
C	0.66797800	2.30845300	-0.02284100
C	1.08838800	0.89239600	-0.02599000
C	2.39956400	0.40820100	0.00268200
C	4.64142400	0.30594600	-0.13294700
C	4.16082500	-0.96049200	0.22668200
N	2.79371100	-0.88005100	0.29765400
N	3.54822100	1.12647100	-0.27454100
C	1.99218300	-1.99128200	0.78487600
H	0.96522800	-1.67042800	0.89485900
H	2.04878600	-2.81471900	0.07264600
H	2.39403300	-2.31995200	1.74308800
C	-2.39961800	0.40842200	-0.00306600
C	-4.16082400	-0.96041900	-0.22677500
C	-4.64145700	0.30601300	0.13295300
N	-3.54832100	1.12664100	0.27425400
N	-2.79378400	-0.87985700	-0.29813000
C	-1.99211400	-1.99092200	-0.78550300
H	-2.04553900	-2.81326100	-0.07174700
H	-2.39619300	-2.32170400	-1.74202900
H	-0.96588200	-1.66894600	-0.89886900
N	-0.00005400	0.07380400	-0.00042200
H	-1.30045900	3.17773500	0.02174200
H	1.30068000	3.17760400	-0.02078700
C	-6.00254900	0.54278900	0.28855400
C	-5.01877800	-2.02988300	-0.45518400
C	-6.37248800	-1.78961200	-0.29891300
C	-6.85421700	-0.52595500	0.06789600
H	-6.38817000	1.51610600	0.55413600
H	-7.91957700	-0.38039000	0.17531000
H	-7.07559700	-2.59330300	-0.46405700
H	-4.64596300	-3.00425500	-0.73591000
C	5.01881000	-2.02982600	0.45550900
C	6.00251500	0.54289400	-0.28816400
C	6.85424400	-0.52574900	-0.06717000
C	6.37255200	-1.78941500	0.29962000
H	4.64601600	-3.00418100	0.73632200
H	7.07570500	-2.59299900	0.46509500
H	7.91962000	-0.38005800	-0.17426000
H	6.38809500	1.51624500	-0.55368700
C	3.62226100	2.45949500	-0.83892100
C	-3.62226000	2.45960000	0.83889400
H	-2.83058300	2.59427300	1.57186700
H	-3.54963100	3.22400600	0.06609000
H	-4.57841700	2.56045100	1.34391700
H	4.57813300	2.56016200	-1.34456000
H	2.83023700	2.59461200	-1.57142000
H	3.55030900	3.22383600	-0.06595200

Compound 4b (Protonated)

Absolute Energy = -1125.058786 a.u.



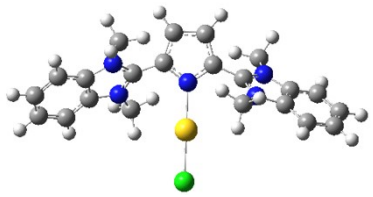
2 1

C	-1.11572200	0.90529000	-0.00557500
C	-0.70368900	2.22025400	-0.00090600
C	0.70364700	2.22027400	0.00123900
C	1.11573100	0.90532400	0.00586200
C	2.47119400	0.37532500	0.03010900
C	4.61012900	0.06727500	-0.45517100
C	4.28596200	-0.75265200	0.62215200
N	2.94536200	-0.52653100	0.90211600
N	3.45122600	0.74771900	-0.80150900
C	2.24673500	-1.10630500	2.04220800
H	1.34402200	-0.53634300	2.24020900
H	2.00408600	-2.14931500	1.84587000
H	2.89736000	-1.04688000	2.91155500
C	-2.47118600	0.37527500	-0.02995000
C	-4.28596100	-0.75248100	-0.62235400
C	-4.61013400	0.06714600	0.45519600
N	-3.45123000	0.74747600	0.80174800
N	-2.94534200	-0.52636000	-0.90219900
C	-2.24678700	-1.10568300	-2.04257000
H	-2.00481100	-2.14897800	-1.84693000
H	-2.89715600	-1.04521900	-2.91203900
H	-1.34366600	-0.53614000	-2.23989000
N	0.00001000	0.10903300	0.00011100
H	-1.34827000	3.08322000	-0.01775400
H	1.34819700	3.08326300	0.01808100
C	-5.89305600	0.10314300	0.99263200
C	-5.22544800	-1.58309500	-1.22487900
C	-6.49764700	-1.54808200	-0.69244100
C	-6.82529300	-0.72038100	0.39647900
H	-6.15151200	0.74244500	1.82458000

H	-7.83794100	-0.72993300	0.77370100
H	-7.26665300	-2.17344100	-1.12304000
H	-4.97891300	-2.22290200	-2.06015300
C	5.22542700	-1.58352500	1.22435800
C	5.89302900	0.10336600	-0.99266000
C	6.82524900	-0.72038900	-0.39680300
C	6.49760200	-1.54841600	0.69186800
H	4.97890400	-2.22360000	2.05942800
H	7.26659100	-2.17395600	1.12223500
H	7.83788400	-0.72987900	-0.77406400
H	6.15148300	0.74292600	-1.82440900
C	3.36784100	1.67991200	-1.92098100
H	0.00000700	-0.89892800	0.00031100
H	3.86096200	1.23065100	-2.77959100
H	2.32622600	1.86887200	-2.15776600
H	3.86459500	2.61263400	-1.66103100
C	-3.36768400	1.67896900	1.92178800
H	-2.32604000	1.86817700	2.15822100
H	-3.86486600	2.61169200	1.66265400
H	-3.86029600	1.22902500	2.78033600

Compound 4b complex with AuCl

Absolute Energy = -1720.375252 a.u.

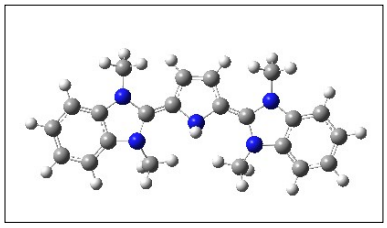


1 1

C	-1.08317800	-1.73427400	0.02590200
C	-0.69719600	-3.07345500	0.00944100
C	0.69831100	-3.07319200	-0.00939100
C	1.08381200	-1.73385900	-0.02611300
C	2.43584200	-1.20130200	-0.06119700
C	4.55666400	-0.82536900	0.47803300
C	4.25438300	-0.08006800	-0.65729700
N	2.93195800	-0.35169800	-0.97104500
N	3.39877200	-1.50556800	0.82280600
C	2.27062800	0.15173900	-2.16748900
H	1.32654500	-0.36762900	-2.29486600
H	2.08596400	1.22024000	-2.06598700
H	2.91754600	-0.03943700	-3.02161400
C	-2.43534800	-1.20192800	0.06099700
C	-4.25408300	-0.08124600	0.65748500
C	-4.55599800	-0.82559700	-0.47856600
N	-3.39795800	-1.50541800	-0.82358900
N	-2.93174800	-0.35309000	0.97140200
C	-2.27058800	0.14977800	2.16816400
H	-2.08636600	1.21842600	2.06736800
H	-2.91738400	-0.04223300	3.02219400
H	-1.32628800	-0.36929200	2.29514200
N	0.00015500	-0.91748600	-0.00019700
H	-1.35042900	-3.93021100	0.03064700
H	1.35184800	-3.92971900	-0.03058300
C	-5.81593700	-0.79343400	-1.06326800
C	-5.19528300	0.73689400	1.26973000
C	-6.44849800	0.77061400	0.68984200
C	-6.75338100	0.01920000	-0.45561100
H	-6.05329800	-1.37214400	-1.94445200
H	-7.74812600	0.08047300	-0.87318500
H	-7.21486100	1.39501600	1.12617700
H	-4.95832200	1.32392900	2.14538100
C	5.19538800	0.73854800	-1.26920200
C	5.81681300	-0.79369300	1.06232400
C	6.75406500	0.01941400	0.45500800
C	6.44881100	0.77176400	-0.68972900
H	4.95813700	1.32631500	-2.14428400
H	7.21504500	1.39648000	-1.12584100
H	7.74896200	0.08030800	0.87227800
H	6.05447700	-1.37312500	1.94295100
C	3.26983900	-2.34023700	2.00678400
C	-3.26855900	-2.33917000	-2.00816500
Au	-0.00043900	1.17567800	0.00015100
Cl	-0.00119000	3.44813600	0.00056100
H	-3.68307000	-1.80197900	-2.85843700
H	-2.21797900	-2.54727600	-2.18155800
H	-3.80964300	-3.27291900	-1.86684900
H	2.21930400	-2.54810100	2.18073500
H	3.81047100	-3.27409000	1.86439700
H	3.68511200	-1.80386300	2.85719300

Compound 4b + Hydride ion

Absolute Energy = -1125.490083 a.u.



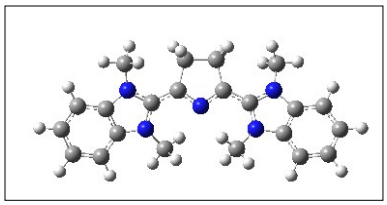
0 1

C	1.15779900	0.84747800	0.25111800
C	0.67560600	2.15267100	0.63800800
C	-0.67458000	2.15325500	0.63869400
C	-1.15820000	0.84853100	0.25232400
C	-2.42978400	0.38808900	0.14096500
C	-4.68715100	0.34820000	-0.13060800
C	-4.22701000	-0.97477200	-0.12607900

N	-2.84283900	-0.94853900	0.00901800
N	-3.58693100	1.17208700	0.03030500
C	-2.17364800	-2.06179200	0.65020300
H	-2.30939700	-2.96207600	0.05183400
H	-1.11547700	-1.84524800	0.73765200
H	-2.58573800	-2.23745100	1.64823300
C	2.42914800	0.38692400	0.13796400
C	4.22741900	-0.97522000	-0.12644400
C	4.68684700	0.34797800	-0.13064600
N	3.58607200	1.17146100	0.02791500
N	2.84257300	-0.94964200	0.00503400
C	2.17289100	-2.06249000	0.64620300
H	2.33461400	-2.96784600	0.06245000
H	2.56327100	-2.22023700	1.65595200
H	1.11011200	-1.85978900	0.70624900
N	-0.00060800	0.01744500	0.05473400
H	1.29616400	2.97163500	0.96015600
H	-1.29411800	2.97270100	0.96159600
C	6.02869200	0.63679500	-0.26881700
C	5.10124300	-2.03647200	-0.21563000
C	6.46460300	-1.74743900	-0.35529900
C	6.91540100	-0.43999500	-0.39005200
H	6.39159600	1.65505900	-0.25998900
H	7.97259900	-0.24112800	-0.49811600
H	7.17222500	-2.56092000	-0.43291700
H	4.74956100	-3.05838200	-0.18775900
C	-5.09970900	-2.03677000	-0.21673400
C	-6.02900000	0.63601500	-0.27052800
C	-6.91469500	-0.44150900	-0.39339900
C	-6.46310000	-1.74866800	-0.35835100
H	-4.74679500	-3.05828500	-0.18869100
H	-7.17008600	-2.56256800	-0.43734800
H	-7.97186600	-0.24336100	-0.50304000
H	-6.39282800	1.65395000	-0.26182700
C	-3.59094700	2.57033800	-0.31283900
C	3.59018400	2.56923800	-0.31725200
H	-0.00152200	-0.43006600	-0.85492600
H	-4.49374400	2.78885100	-0.88057800
H	-3.56962400	3.21490600	0.56787500
H	-2.72195400	2.79411300	-0.93251700
H	3.57041500	3.21519000	0.56250700
H	4.49226800	2.78653800	-0.88665200
H	2.72040600	2.79242000	-0.93598600

Compound 4b (ASE)

Absolute Energy = -1125.934241 a.u.



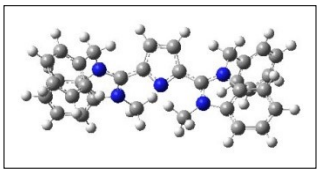
1 1

C	-1.09236700	1.04822200	0.04306700
C	-0.75908900	2.52977100	0.14287200
C	0.75906700	2.52981300	-0.14295400
C	1.09240200	1.04826700	-0.04326700
C	2.37297800	0.45602000	0.00083500
C	4.59114600	0.16539500	-0.16055100
C	4.03104800	-1.01538400	0.32341900
N	2.66351000	-0.80085900	0.42716600
N	3.54214500	1.05530000	-0.35373600
C	1.74283600	-1.75282600	1.01772900
H	1.03460800	-1.22915800	1.65204600
H	1.19344200	-2.29112900	0.24778900
H	2.32193800	-2.45197400	1.61419600
C	-2.37294200	0.45596900	-0.00098300
C	-4.03110500	-1.01536500	-0.32339900
C	-4.59110400	0.16543300	0.16064200
N	-3.54204600	1.05529900	0.35369500
N	-2.66357200	-0.80089300	-0.42731500
C	-1.74302800	-1.75290600	-1.01801000
H	-1.19353300	-2.29121800	-0.24814900
H	-2.32226100	-2.45204200	-1.61436800
H	-1.03488100	-1.22928300	-1.65245200
N	0.00003200	0.29433500	-0.00010400
H	-1.30688200	3.14206800	-0.57049100
H	1.30682800	3.14207700	0.57046000
C	-5.95618800	0.28708500	0.36982100
C	-4.81218100	-2.12338500	-0.61418400
C	-6.17706300	-2.00258200	-0.40626000
C	-6.73857200	-0.81896900	0.07723200
H	-6.40270500	1.19944000	0.73747000
H	-7.80714900	-0.76268000	0.22714100
H	-6.81984600	-2.84419600	-0.62080500
H	-4.38409100	-3.04576600	-0.97864800
C	4.81204700	-2.12343400	0.61429500
C	5.95625900	0.28699700	-0.36956700
C	6.73856900	-0.81908800	-0.07688500
C	6.17695800	-2.00268100	0.40653500
H	4.38388000	-3.04580300	0.97870100
H	6.81968500	-2.84432000	0.62115200
H	7.80716500	-0.76283800	-0.22666800
H	6.40285500	1.19933500	-0.73716100
C	3.67666200	2.32863400	-1.03986700
C	-3.67640300	2.32865200	1.03982100
H	-3.01796700	2.35761200	1.90459500

H	-3.45702500	3.16250700	0.37794900
H	-4.70095600	2.41748000	1.38550600
H	4.70127900	2.41741400	-1.38537500
H	3.01838900	2.35759800	-1.90476100
H	3.45720200	3.16251400	-0.37805300
H	-0.95903400	2.92405900	1.13978400
H	0.95899000	2.92419100	-1.13983400

Compound 4c (Singlet)

Absolute Energy = -1586.711893 a.u.

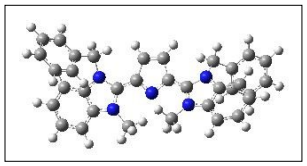


1 1

C	-0.98612200	0.40982600	0.74054200
C	-0.64028800	0.26134100	2.10094700
C	0.64024600	-0.26148800	2.10094500
C	0.98611000	-0.40988800	0.74053900
C	2.19679600	-0.96333900	0.18622300
C	4.33659300	-1.48434700	-0.15015600
C	3.57722200	-2.09742900	-1.14150000
N	2.25391100	-1.75869700	-0.89593200
N	3.44736800	-0.78382900	0.65519600
C	1.12901000	-2.28043100	-1.65575900
H	0.24442100	-2.27188500	-1.02968200
H	0.94705200	-1.66404100	-2.53331000
H	1.36872300	-3.29739200	-1.95706300
C	3.87141800	0.14279800	1.70284300
C	-2.19679400	0.96331600	0.18623500
C	-3.57718900	2.09750200	-1.14143800
C	-4.33658300	1.48435500	-0.15015200
N	-3.44737700	0.78377900	0.65517000
N	-2.25388400	1.75874700	-0.89586800
C	-3.87145300	-0.14291500	1.70274700
C	-1.12896900	2.28053200	-1.65563700
H	-0.94702500	1.66422600	-2.53325100
H	-1.36865600	3.29752900	-1.95684000
H	-0.24438200	2.27190000	-1.02955900
N	0.00000300	-0.00000600	-0.08368100
H	-1.22761600	0.53434600	2.96232900
H	1.22755300	-0.53454700	2.96232400
C	-5.71709100	1.62096100	-0.09726300
C	-4.15903600	2.88519200	-2.12544300
C	-5.53359500	3.02959900	-2.07023500
C	-6.29851500	2.40783300	-1.07496300
H	-6.30791100	1.12814600	0.66126000
H	-7.37064100	2.54285300	-1.07455000
H	-6.03091500	3.63369800	-2.81556900
H	-3.57278700	3.35848100	-2.89984400
C	4.15909300	-2.88504800	-2.12554800
C	5.71710100	-1.62095000	-0.09724800
C	6.29854800	-2.40775200	-1.07499200
C	5.53365200	-3.02945200	-2.07032200
H	3.57286200	-3.35828500	-2.89999400
H	6.03099000	-3.63349600	-2.81568900
H	7.37067500	-2.54276600	-1.07456600
H	6.30790300	-1.12818400	0.66132100
C	-4.78364800	-1.22095600	1.16639700
C	-4.48294600	-1.86761100	-0.02759600
C	-5.91167600	-1.59743400	1.88316600
C	-5.30465600	-2.87863200	-0.50007100
H	-3.60459900	-1.57658000	-0.59293000
C	-6.73239300	-2.61472400	1.41374000
H	-6.15267400	-1.09463400	2.81225400
C	-6.43097300	-3.25458300	0.22102200
H	-5.06781900	-3.37483900	-1.43121400
H	-7.60916400	-2.90155600	1.97776100
H	-7.07245400	-4.04258200	-0.14838500
C	4.78361700	1.22088100	1.16658200
C	4.48293100	1.86761200	-0.02737400
C	5.91162900	1.59731900	1.88339500
C	5.30464300	2.87866900	-0.49976900
H	3.60459600	1.57661200	-0.59274300
C	6.73234800	2.61464500	1.41405000
H	6.15261500	1.09446000	2.81245300
C	6.43094500	3.25458100	0.22136800
H	5.06781800	3.37493600	-1.43088300
H	7.60910700	2.90144700	1.97810500
H	7.07242700	4.04260800	-0.14797600
H	2.97131300	0.58375300	2.12321200
H	4.36926700	-0.42827500	2.48707500
H	-2.97135900	-0.58390300	2.12310500
H	-4.36931400	0.42810900	2.48700800

Compound 4c (Triplet)

Absolute Energy = -1586.607488 a.u.



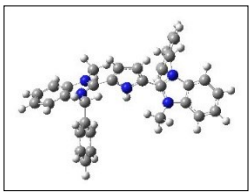
1 3

C	-1.04728400	0.28275000	0.33236100
C	-0.64704700	0.16045100	1.74887100
C	0.64713700	-0.17517000	1.74822600
C	1.04851700	-0.28759000	0.33113600
C	2.29105000	-0.70484500	-0.15532300
C	4.43956600	-1.34338500	-0.27184700

C	3.82460500	-1.64454600	-1.49576400
N	2.51677900	-1.22746700	-1.41064500
N	3.49118400	-0.74848000	0.52985000
C	1.50902800	-1.50063300	-2.42238100
H	0.65971300	-2.00781500	-1.97464200
H	1.16423200	-0.57467100	-2.87342900
H	1.95916800	-2.13730400	-3.17708500
C	3.83548100	0.00794800	1.73162500
C	-2.28942300	0.70373500	-0.15225100
C	-3.82167300	1.65279900	-1.48741800
C	-4.43787600	1.34288300	-0.26633700
N	-3.49017700	0.74208200	0.53188900
N	-2.51381800	1.23536900	-1.40385800
C	-3.83448000	-0.02140300	1.72922600
C	-1.50514800	1.51576000	-2.41271400
H	-1.16112800	0.59317700	-2.87124900
H	-1.95412700	2.15922100	-3.16233900
H	-0.65555700	2.01821300	-1.96024100
N	0.00089100	0.00044200	-0.49123300
H	-1.25465900	0.35548400	2.61565400
H	1.25402000	-0.37636400	2.61410600
C	-5.77879500	1.62753600	-0.03491800
C	-4.52765500	2.27346900	-2.51354300
C	-5.85836900	2.56474500	-2.27511600
C	-6.47416000	2.24724100	-1.05723800
H	-6.25656700	1.37197700	0.89916600
H	-7.51743800	2.49000800	-0.91508000
H	-6.43864900	3.04675700	-3.04890500
H	-4.06795600	2.51482800	-3.46024800
C	4.53175500	-2.25785300	-2.52552300
C	5.78036400	-1.62912400	-0.04119100
C	6.47688800	-2.24143900	-1.06716200
C	5.86229300	-2.55054700	-2.28781400
H	4.07309500	-2.49259900	-3.47439200
H	6.44344000	-3.02695300	-3.06441800
H	7.52011700	-2.48486600	-0.92578600
H	6.25714500	-1.37985100	0.89511000
C	-4.97314100	-0.98964900	1.50062100
C	-5.00427200	-1.78540500	0.36060600
C	-5.97604200	-1.11636000	2.45192100
C	-6.03084800	-2.69730000	0.17448500
H	-4.22644500	-1.68594900	-0.38833000
C	-7.00288200	-2.03363900	2.26892500
H	-5.95937000	-0.49460500	3.33921100
C	-7.03211500	-2.82333900	1.12972300
H	-6.05152700	-3.31096700	-0.71559200
H	-7.78111300	-2.12542800	3.01397200
H	-7.83351700	-3.53410500	0.98330900
C	4.97103100	0.98088900	1.50723600
C	4.99868700	1.78293800	0.37154300
C	5.97449800	1.10539800	2.45823200
C	6.02231700	2.69896100	0.18945200
H	4.22046700	1.68524600	-0.37722300
C	6.99836900	2.02678400	2.27929300
H	5.96058300	0.47874900	3.34212400
C	7.02410300	2.82282500	1.14441700
H	6.04028500	3.31752000	-0.69729500
H	7.77705900	2.11682700	3.02407400
H	7.82321000	3.53681100	1.00115600
H	2.95267600	0.56609200	2.02683300
H	4.08309400	-0.68828500	2.53488900
H	-2.95264800	-0.58410600	2.01871500
H	-4.07848100	0.67000200	2.53776000

Compound 4c (Protonated)

Absolute Energy = -1586.997541 a.u.



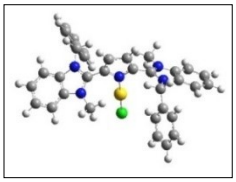
2 1

C	-1.01473300	0.46039400	1.24320900
C	-0.64277500	0.29025200	2.55627200
C	0.64275200	-0.29083600	2.55626500
C	1.01481600	-0.46071300	1.24319800
C	2.24104200	-1.03608900	0.69675000
C	4.37202200	-1.33256500	0.18035400
C	3.64956800	-2.41752600	-0.30918000
N	2.32333400	-2.19735800	0.03415700
N	3.45916600	-0.49717600	0.80705900
C	1.24466900	-3.14497400	-0.21536900
H	0.34442800	-2.80478900	0.28770500
H	1.06712700	-3.22714400	-1.28579100
H	1.53187400	-4.11660600	0.18065200
C	3.80115700	0.80517300	1.38012700
C	-2.24090500	1.03589800	0.69678000
C	-3.64930300	2.41751500	-0.30908600
C	-4.37185500	1.33259200	0.18038600
N	-3.45907700	0.49708400	0.80704800
N	-2.32309000	2.19721300	0.03425000
C	-3.80119800	-0.80526600	1.38004000
C	-1.24434800	3.14476100	-0.21520000
H	-1.06674500	3.22694900	-1.28561000
H	-1.53151000	4.11640200	0.18083100
H	-0.34415500	2.80450700	0.28791300
N	0.00007500	-0.00007700	0.44654500
H	-1.22866000	0.56528100	3.41740600
H	1.22857100	-0.56603200	3.41739100
C	-5.74787100	1.22297100	0.00205200
C	-4.26298200	3.46576500	-0.98861500
C	-5.62790400	3.36279300	-1.15639300

C	-6.35635500	2.26017600	-0.67242400
H	-6.30457600	0.36931200	0.36184700
H	-7.42366000	2.22702500	-0.83843800
H	-6.15583100	4.14917400	-1.67678500
H	-3.70674200	4.31249500	-1.36475000
C	4.26334400	-3.46568400	-0.98876400
C	5.74802800	-1.22281000	0.00203000
C	6.35660800	-2.25992200	-0.67250100
C	5.62825800	-3.36257900	-1.15653100
H	3.70718200	-4.31244400	-1.36494700
H	6.15625800	-4.14888500	-1.67696400
H	7.42391000	-2.22666600	-0.83851000
H	6.30465500	-0.36912000	0.36187400
C	-4.23685900	-1.79824700	0.32718500
C	-3.74356700	-1.74964600	-0.97147700
C	-5.12644100	-2.80449200	0.68605000
C	-4.13429300	-2.70133600	-1.90340700
H	-3.07229700	-0.95322800	-1.27488800
C	-5.51048600	-3.76027200	-0.24333900
H	-5.52403600	-2.84222300	1.69311900
C	-5.01529100	-3.70978000	-1.53903000
H	-3.76115700	-2.64924800	-2.91699900
H	-6.20514000	-4.53774500	0.04248800
H	-5.32451000	-4.44753700	-2.26609600
C	4.23662400	1.79829100	0.32732000
C	3.74333200	1.74967200	-0.97134100
C	5.12602700	2.80467800	0.68623400
C	4.13388000	2.70148600	-1.90322200
H	3.07221300	0.95314400	-1.27479700
C	5.50989200	3.76057800	-0.24310500
H	5.52362300	2.84242400	1.69330100
C	5.01469700	3.71006900	-1.53879600
H	3.76075000	2.64938200	-2.91681600
H	6.20441000	4.53815900	0.04275900
H	5.32378100	4.44792000	-2.26582400
H	2.92450600	1.15774800	1.92145700
H	4.59572900	0.64219100	2.10827200
H	-2.92455600	-1.15799600	1.92128500
H	-4.59570300	-0.64223900	2.10824800
H	0.00011700	0.00002400	-0.56158100

Compound 4c complex with AuCl

Absolute Energy = -2182.305366 a.u.

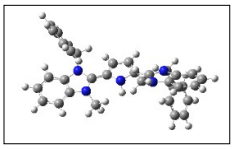


1 1			
C	0.99538700	0.46170500	-1.75285200
C	0.63946200	0.29059600	-3.09873500
C	-0.63913000	-0.29123400	-3.09883400
C	-0.99550100	-0.46177200	-1.75300300
C	-2.21740800	-1.05510100	-1.21589000
C	-4.37358900	-1.39225700	-0.72076100
C	-3.62941100	-2.47003200	-0.21595800
N	-2.29870800	-2.23036900	-0.55166100
N	-3.46152200	-0.53075200	-1.33274600
C	-1.19082300	-3.13783600	-0.24904500
H	-0.30704300	-2.81065300	-0.79348400
H	-0.98031900	-3.12190700	0.82311000
H	-1.46448600	-4.14721700	-0.56474500
C	-3.79806800	0.77946500	-1.91997500
C	2.21710700	1.05524700	-1.21563600
C	3.62874800	2.47031100	-0.21536400
C	4.37323900	1.39298300	-0.72064800
N	3.46139900	0.53137500	-1.33283600
N	2.29808600	2.23031800	-0.55099400
C	3.79832100	-0.77866800	-1.92026200
C	1.19000200	3.13745400	-0.24813900
H	0.97969600	3.12140300	0.82405100
H	1.46332600	4.14693800	-0.56381600
H	0.30620800	2.81005400	-0.79241400
N	-0.00021300	0.00014900	-0.93075800
H	1.22798000	0.57329900	-3.96123700
H	-1.22740100	-0.57421700	-3.96141200
C	5.76085600	1.32472000	-0.56375700
C	4.23368200	3.52926400	0.46772200
C	5.61577700	3.46371400	0.61984100
C	6.36518600	2.38081800	0.11254900
H	6.33842800	0.48636300	-0.93440700
H	7.44001200	2.36752600	0.26038500
H	6.12924500	4.26188800	1.14567200
H	3.65974500	4.35814700	0.86677300
C	-4.23463800	-3.52901800	0.46682100
C	-5.76116900	-1.32357000	-0.56370100
C	-6.36578600	-2.37970500	0.11228300
C	-5.61669200	-3.46304200	0.61910900
H	-3.66094600	-4.35823900	0.86552400
H	-6.13037800	-4.26122100	1.14472000
H	-7.44059200	-2.36609900	0.26024500
H	-6.33848300	-0.48487400	-0.93398700
C	4.33831200	-1.77113400	-0.90548700
C	3.72944800	-1.93889500	0.34622500
C	5.43781600	-2.56917400	-1.24601100
C	4.22006200	-2.88780300	1.24579500
H	2.87849200	-1.32581000	0.63367900
C	5.92197700	-3.52662400	-0.34952800
H	5.91878600	-2.44723100	-2.21402200
C	5.31560500	-3.68511200	0.89898100
H	3.74723900	-2.99998700	2.21685700

H	6.77513200	-4.13948300	-0.62442600
H	5.69668200	-4.42146600	1.60001100
C	-4.33778300	1.77194700	-0.90507400
C	-3.72914000	1.93911100	0.34682400
C	-5.43682800	2.57058900	-1.24567000
C	-4.21951100	2.88804900	1.24649500
H	-2.87855500	1.32554100	0.63433500
C	-5.92073300	3.52807100	-0.34908400
H	-5.91764800	2.44908300	-2.21381000
C	-5.31457900	3.68598000	0.89960400
H	-3.74687300	2.99977700	2.21769900
H	-6.77353500	4.14139700	-0.62403800
H	-5.69546700	4.42235400	1.60071400
H	-2.88240800	1.14708800	-2.38865900
H	-4.52867800	0.60894500	-2.71668200
H	2.88277100	-1.14650300	-2.38898700
H	4.52887800	-0.60783100	-2.71694600
Au	0.00000600	-0.00051500	1.14097400
Cl	0.00030700	-0.00151300	3.44719300

Compound 4c + Hydride ion

Absolute Energy = -1587.412351 a.u.

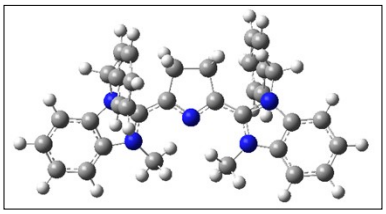


0 1

C	-1.02745600	-0.47058100	-0.39797900
C	-0.60302900	-0.44720500	-1.78056100
C	0.67098100	-0.00846800	-1.85927900
C	1.15231300	0.29711400	-0.53423000
C	2.33442600	0.81158400	-0.11557100
C	4.49652900	1.50109900	-0.02992600
C	3.89154700	1.83199700	1.18643400
N	2.57512900	1.37614600	1.14710800
N	3.54382700	0.87484300	-0.82859700
C	1.52099100	2.02280000	1.90657300
H	0.80998700	2.49463800	1.22778200
H	0.97605400	1.31625400	2.52911100
H	1.97252200	2.78134400	2.54089700
C	3.95581800	-0.09374900	-1.82241200
C	-2.25840400	-0.75533800	0.09294900
C	-3.90586500	-1.48937500	1.47697700
C	-4.41736300	-1.45885000	0.17690300
N	-3.42354700	-0.96946600	-0.67050600
N	-2.60847600	-0.97919200	1.43617300
C	-3.80122700	-0.13116500	-1.79909800
C	-1.63575900	-1.31884000	2.44857600
H	-0.99609600	-0.46896700	2.67249100
H	-2.16045500	-1.59550800	3.35820200
H	-1.02325000	-2.16978500	2.13141000
N	0.08967100	-0.01136500	0.39016100
H	-1.20684900	-0.75237600	-2.61874100
H	1.21117500	0.15809300	-2.77663300
C	-5.71603600	-1.83034200	-0.09400800
C	-4.67391500	-1.94125000	2.53110700
C	-5.98372900	-2.34579400	2.25547000
C	-6.49895200	-2.28322300	0.97175100
H	-6.11718700	-1.77029400	-1.09649200
H	-7.51995300	-2.58679400	0.78793600
H	-6.60419900	-2.70509800	3.06466500
H	-4.29330100	-1.97090400	3.54228300
C	4.59862400	2.48082800	2.17743600
C	5.82701400	1.76995300	-0.26900500
C	6.54659100	2.42523600	0.73489600
C	5.94187500	2.78122400	1.92865700
H	4.14207700	2.73476100	3.12389200
H	6.51725200	3.29004600	2.68947100
H	7.59117800	2.65235600	0.57444300
H	6.29983300	1.48129800	-1.19776900
C	-4.77454800	0.97223200	-1.44002200
C	-4.64367900	1.67070800	-0.24336000
C	-5.79182800	1.32024000	-2.31854700
C	-5.51514300	2.70392800	0.06278000
H	-3.86021400	1.39625700	0.45394500
C	-6.66391400	2.35822600	-2.01604200
H	-5.90704700	0.77179200	-3.24632600
C	-6.52667400	3.05248100	-0.82385200
H	-5.40740000	3.23801000	0.99732100
H	-7.45398000	2.61745900	-2.70809600
H	-7.20758900	3.85724300	-0.58192200
C	4.79886500	-1.22585900	-1.26896400
C	4.64807200	-1.66525200	0.04149200
C	5.71592500	-1.86524200	-2.09474500
C	5.39873100	-2.73198000	0.51374900
H	3.94736300	-1.16472900	0.69910900
C	6.46550000	-2.93490400	-1.62573100
H	5.84751800	-1.52040100	-3.11394900
C	6.30747800	-3.37154300	-0.31838100
H	5.27677300	-3.06222300	1.53663400
H	7.17747200	-3.42150300	-2.27891900
H	6.89418500	-4.20089700	0.05266900
H	3.06411100	-0.51175900	-2.27995200
H	4.50772800	0.42064700	-2.61219200
H	-2.89523800	0.31827900	-2.19543200
H	-4.22599700	-0.75533500	-2.58833500
H	0.40474800	-0.69281400	1.06789900

Compound 4c (ASE)

Absolute Energy = -1587.869076



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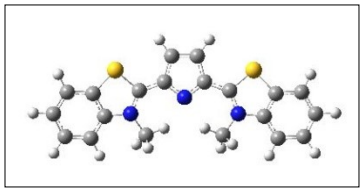
C	-1.04159800	-0.33183300	-0.39884900
C	-0.75895000	-0.14352100	-1.87948200
C	0.75904700	0.14278100	-1.87952900
C	1.04167100	0.33166300	-0.39896400
C	2.24133900	0.76393100	0.20360000
C	4.40734800	1.24627300	0.54340800
C	3.71599700	1.49232500	1.72778300
N	2.38044400	1.20463500	1.48260400
N	3.46879900	0.81795500	-0.38847500
C	1.31853400	1.46977300	2.43311600
H	0.45157800	1.86110600	1.91043300
H	1.03147000	0.56071900	2.95840300
H	1.68275500	2.20654900	3.14387500
C	3.83619600	0.22012800	-1.66140200
C	-2.24128200	-0.76387400	0.20385400
C	-3.71599800	-1.49172900	1.72824300
C	-4.40730300	-1.24611400	0.54375100
N	-3.46872400	-0.81810900	-0.38824400
N	-2.38043500	-1.20412800	1.48301100
C	-3.83608900	-0.22067400	-1.66136700
C	-1.31857200	-1.46894100	2.43366700
H	-1.03145400	-0.55968500	2.95857300
H	-1.68287600	-2.20538300	3.14473000
H	-0.45163200	-1.86057600	1.91118700
N	0.00002900	0.00006900	0.35545700
H	-1.00135700	-1.02339100	-2.47306700
H	1.00145900	1.02242500	-2.47344900
C	-5.77946000	-1.42320300	0.45642800
C	-4.36465900	-1.93936000	2.86876800
C	-5.73520700	-2.12770300	2.77940300
C	-6.43003200	-1.87066800	1.59603700
H	-6.32876900	-1.22034100	-0.45136100
H	-7.49982600	-2.01971600	1.56721100
H	-6.27785500	-2.47383400	3.64732700
H	-3.83579100	-2.12448100	3.79235500
C	4.36461500	1.94037200	2.86816900
C	5.77950800	1.42332700	0.45607400
C	6.43003700	1.87120800	1.59554300
C	5.73516600	2.12867800	2.77878800
H	3.83571100	2.12583000	3.79167000
H	6.27778300	2.47512500	3.64660600
H	7.49983300	2.02024300	1.56670400
H	6.32885300	1.22013000	-0.45162000
C	-3.84138800	1.29212300	-1.64093200
C	-3.91688900	2.01148800	-0.45546400
C	-3.79892100	1.97522000	-2.85295800
C	-3.95164400	3.40012700	-0.48240500
H	-3.95799800	1.49493900	0.49587900
C	-3.83643300	3.36042400	-2.87982900
H	-3.73641300	1.41917100	-3.78142800
C	-3.91216800	4.07648000	-1.69198400
H	-4.01530900	3.95231700	0.44523700
H	-3.80542700	3.88117200	-3.82701700
H	-3.94154300	5.15706700	-1.71106000
C	3.84140800	-1.29266000	-1.64052300
C	3.91673700	-2.01169200	-0.45484300
C	3.79902100	-1.97609900	-2.85236000
C	3.95140900	-3.40034000	-0.48138500
H	3.95778000	-1.49487100	0.49635600
C	3.83644900	-3.36131200	-2.87883300
H	3.73664100	-1.42031000	-3.78099400
C	3.91201800	-4.07703400	-1.69077500
H	4.01494300	-3.95227000	0.44642000
H	3.80550900	-3.88232800	-3.82587600
H	3.94132700	-5.15762800	-1.70954100
H	3.17520100	0.58845400	-2.44171000
H	4.83006200	0.59621300	-1.90087900
H	-3.17505000	-0.58919900	-2.44154400
H	-4.82993000	-0.59687600	-1.90076600
H	-1.31353400	0.70435000	-2.28594900
H	1.31363800	-0.70524400	-2.28566700

Compound 4d (Singlet)

Absolute Energy = -1731.895738 a.u.



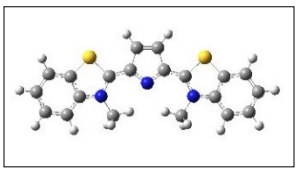
1 1

C	1.06762400	1.01134400	0.02409300
C	0.68439000	2.38220400	0.00934800
C	-0.68439400	2.38220200	-0.00929900
C	-1.06762200	1.01134000	-0.02405400
C	-2.41965400	0.54843900	-0.02604400
C	-4.87995400	0.39004000	0.16065800
C	-4.26003300	-0.81177800	-0.17076700
N	-2.87349500	-0.67753200	-0.28401400
C	-2.05730600	-1.81288900	-0.70872700
H	-1.08412200	-1.45320900	-1.01455100
H	-1.94542700	-2.51065600	0.12040300

H	-2.56513600	-2.30316200	-1.53567000
C	2.41965600	0.54844600	0.02607500
C	4.26003600	-0.81177400	0.17077000
C	4.87994900	0.39003800	-0.16069000
N	2.87350100	-0.67752200	0.28406200
C	2.05731700	-1.81286100	0.70883300
H	1.94524500	-2.51056400	-0.12032500
H	2.56526100	-2.30322000	1.53565400
H	1.08420800	-1.45314700	1.01485300
N	0.00000200	0.18988400	-0.00000500
H	1.33590500	3.24120700	0.02774100
H	-1.33591100	3.24120300	-0.02767500
C	6.25872200	0.47197100	-0.30641100
C	5.00322500	-1.97246200	0.35517300
C	6.37536900	-1.88860600	0.20705200
C	6.99792500	-0.68095200	-0.11742100
H	6.73637700	1.40703700	-0.56188100
H	8.07247600	-0.64690700	-0.22604700
H	6.97595600	-2.77651200	0.34363300
H	4.52990000	-2.91233900	0.59850600
C	-5.00321600	-1.97246700	-0.35518500
C	-6.25873100	0.47197500	0.30633300
C	-6.99793000	-0.68094900	0.11733200
C	-6.37536600	-1.88860800	-0.20710900
H	-4.52988400	-2.91234500	-0.59849800
H	-6.97595000	-2.77651300	-0.34370200
H	-8.07248400	-0.64690200	0.22592400
H	-6.73639400	1.40704500	0.56177800
S	-3.69423400	1.63804000	0.35841700
S	3.69422700	1.63803900	-0.35843100

Compound 4d (Triplet)

Absolute Energy = -1731.819025 a.u.

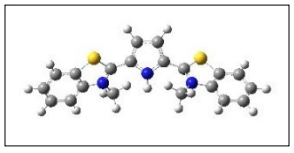


1 3

C	-1.07931900	0.88076700	-0.01620100
C	-0.66659000	2.30072900	-0.00785100
C	0.66659000	2.30072900	0.00785500
C	1.07931900	0.88076600	0.01620600
C	2.41888000	0.49018100	0.03521500
C	4.89664700	0.46739200	-0.02824700
C	4.31842200	-0.80790500	0.03531800
N	2.94210100	-0.77391500	0.08046700
C	2.17948900	-2.00979400	0.20774400
H	1.13545500	-1.76510500	0.34513800
H	2.30866100	-2.60965300	-0.69329200
H	2.55322800	-2.56468500	1.06741100
C	-2.41888100	0.49018300	-0.03521300
C	-4.31842200	-0.80790500	-0.03531900
C	-4.89664700	0.46739200	0.02824400
N	-2.94210000	-0.77391400	-0.08046500
C	-2.17948700	-2.00979200	-0.20773900
H	-2.30866000	-2.60965000	0.69329700
H	-2.55322200	-2.56468500	-1.06740600
H	-1.13545300	-1.76510100	-0.34513000
N	-0.00000100	0.05873900	0.00000300
H	-1.32363500	3.15566300	-0.01711500
H	1.32363600	3.15566200	0.01711600
C	-6.27596900	0.63079600	0.07414400
C	-5.12211400	-1.94887300	-0.05133600
C	-6.49080600	-1.77782400	-0.00395000
C	-7.06555300	-0.50258600	0.05714400
H	-6.71478200	1.61719200	0.12176500
H	-8.14088000	-0.40328500	0.09250400
H	-7.13200800	-2.64779800	-0.01321500
H	-4.68792000	-2.93687100	-0.09419700
C	5.12211500	-1.94887200	0.05133500
C	6.27596900	0.63079700	-0.07415000
C	7.06555200	-0.50258400	-0.05715000
C	6.49080700	-1.77782200	0.00394600
H	4.68792200	-2.93687100	0.09419700
H	7.13201000	-2.64779600	0.01321000
H	8.14088000	-0.40328300	-0.09251400
H	6.71478100	1.61719400	-0.12177200
S	3.67775000	1.68931400	-0.03615600
S	-3.67775100	1.68931500	0.03615600

Compound 4d (Protonated)

Absolute Energy = -1732.160618 a.u.



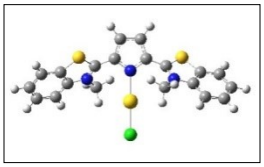
2 1

C	1.11484500	0.99525600	0.00161100
C	0.70178200	2.31236700	-0.00873900
C	-0.70178300	2.31236700	0.00873200
C	-1.11484500	0.99525600	-0.00160900
C	-2.48303200	0.50878800	0.03983400
C	-4.86109300	0.17797300	0.52377600
C	-4.36210500	-0.68432600	-0.45364600
N	-3.00943500	-0.45050200	-0.70912400
C	-2.31709800	-1.15098400	-1.79254500

H	-1.39607300	-0.62854500	-2.02832400
H	-2.11671600	-2.18054700	-1.50006300
H	-2.96019300	-1.14342900	-2.66914000
C	2.48303200	0.50878900	-0.03983300
C	4.36210600	-0.68432300	0.45364800
C	4.86109100	0.17797100	-0.52378000
N	3.00943700	-0.45049700	0.70913000
C	2.31710300	-1.15097200	1.79255700
H	2.11671800	-2.18053600	1.50008100
H	2.96020100	-1.14341400	2.66914900
H	1.39607900	-0.62853100	2.02833600
N	0.00000000	0.19575200	0.00000400
H	1.34899400	3.17368300	-0.00559300
H	-1.34899600	3.17368200	0.00558000
C	6.19667800	0.12961300	-0.91542200
C	5.17943500	-1.62930000	1.07011500
C	6.50032300	-1.67430300	0.67705100
C	7.00386900	-0.80543900	-0.30220700
H	6.58440400	0.79811600	-1.67073200
H	8.04566700	-0.87076000	-0.58245800
H	7.16285700	-2.39544000	1.13426600
H	4.80083300	-2.30524700	1.82338200
C	-5.17943200	-1.62930700	-1.07011000
C	-6.19668100	0.12961800	0.91541400
C	-7.00387000	-0.80543800	0.30220100
C	-6.50032200	-1.67430700	-0.67705000
H	-4.80082800	-2.30525800	-1.82337200
H	-7.16285400	-2.39544600	-1.13426300
H	-8.04566900	-0.87075700	0.58244900
H	-6.58441000	0.79812500	1.67071900
S	-3.60248000	1.20927400	1.10783300
S	3.60247700	1.20926800	-1.10783900
H	0.00000100	-0.81144000	0.00000800

Compound 4d complex with AuCl

Absolute Energy = -2327.481549 a.u.

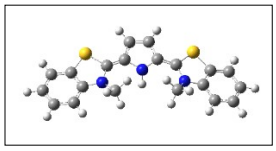


1 1

C	-1.08233800	1.79554800	-0.00474600
C	-0.69571000	3.13828100	0.01522200
C	0.69466800	3.13845800	-0.01278900
C	1.08144000	1.79574400	0.00530600
C	2.44261700	1.29994900	-0.02485900
C	4.79949900	0.87119200	-0.57599300
C	4.32171600	0.11487100	0.49246700
N	2.98931600	0.40738800	0.78697900
C	2.35699600	-0.14715400	1.98645600
H	1.40917700	0.35271100	2.15038200
H	2.19160800	-1.21539100	1.85412200
H	3.02556900	0.03152100	2.82640400
C	-2.44331800	1.29963200	0.02486800
C	-4.32201700	0.11398300	-0.49276700
C	-4.80046500	0.87079500	0.57504700
N	-2.98952000	0.40652700	-0.78677300
C	-2.35675800	-0.14798400	-1.98603800
H	-2.19102800	-1.21615300	-1.85357300
H	-3.02524900	0.03029500	-2.82613300
H	-1.40906000	0.35213300	-2.14983000
N	-0.00028600	0.97511600	-0.00033800
H	-1.35288900	3.99195100	0.01748200
H	1.35173400	3.99220900	-0.01401000
C	-6.11555300	0.74424800	1.01159400
C	-5.13782200	-0.79952700	-1.15393300
C	-6.43964200	-0.92463700	-0.71405700
C	-6.92447000	-0.16064800	0.35459300
H	-6.48731400	1.33059300	1.83956000
H	-7.94927900	-0.28500400	0.67410600
H	-7.09677700	-1.62978100	-1.20253000
H	-4.76425900	-1.39810600	-1.97208100
C	5.13796500	-0.79818600	1.15371800
C	6.11439900	0.74458600	-1.01313600
C	6.92375200	-0.15985600	-0.35606700
C	6.43956600	-0.92335500	0.71324200
H	4.76489000	-1.39637900	1.97237200
H	7.09704400	-1.62815900	1.20174400
H	7.94841600	-0.28424700	-0.67602900
H	6.48566000	1.33053400	-1.84160800
S	3.53603800	1.87711100	-1.19933000
S	-3.53746700	1.87721400	1.19854400
Au	0.00040300	-1.12005200	0.00005300
Cl	0.00170900	-3.39192200	0.00118700

Compound 4d + Hydride ion

Absolute Energy = -1732.647197 a.u.

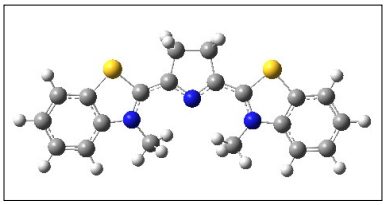


0 1

C	-1.15003000	-1.03569000	0.26852700
C	-0.67383900	-2.39841600	0.29739900
C	0.67383600	-2.39842800	0.29740600
C	1.15004600	-1.03571000	0.26852000
C	2.43048200	-0.61533800	0.21206200

C	4.88329300	-0.38431900	-0.27558600
C	4.23146800	0.83876700	-0.07750800
N	2.89109500	0.70532400	0.24063200
C	2.19409800	1.76870200	0.93802300
H	1.38983900	1.34215800	1.52846400
H	2.89100100	2.27757400	1.60561700
H	1.77721300	2.50524800	0.24614500
C	-2.43046600	-0.61531300	0.21207600
C	-4.23147600	0.83876300	-0.07750500
C	-4.88328100	-0.38433000	-0.27559600
N	-2.89110200	0.70534300	0.24063700
C	-2.19414900	1.76876500	0.93800400
H	-1.77752700	2.50544100	0.24610700
H	-2.89100700	2.27746400	1.60578100
H	-1.38970700	1.34230100	1.52825000
N	0.00001600	-0.19414400	0.31727300
H	-1.31632500	-3.26425300	0.33214000
H	1.31630800	-3.26427500	0.33215200
C	-6.22875800	-0.43289200	-0.57492100
C	-4.94035100	2.02703200	-0.17759300
C	-6.29875500	1.97452900	-0.48207300
C	-6.93939000	0.76242000	-0.68065900
H	-6.72406200	-1.38336300	-0.71900100
H	-7.99357400	0.73772800	-0.91743700
H	-6.85580100	2.89746500	-0.56660300
H	-4.44452300	2.97728800	-0.03560900
C	4.94032400	2.02704600	-0.17761800
C	6.22877300	-0.43286300	-0.57490200
C	6.93938800	0.76245800	-0.68064800
C	6.29873100	1.97456000	-0.48208500
H	4.44447900	2.97729700	-0.03566300
H	6.85576200	2.89750400	-0.56663000
H	7.99357400	0.73777900	-0.91741900
H	6.72409100	-1.38332800	-0.71897000
S	3.78287600	-1.72851900	-0.04845600
S	-3.78284400	-1.72851100	-0.04845800
H	0.00002300	0.55834300	-0.35843800

Compound 4d (ASE)



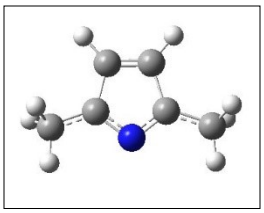
Absolute Energy = -1733.066263 a.u.

1 1

C	-1.08553900	1.04428900	-0.03124900
C	-0.76958300	2.52616800	0.03729700
C	0.76957500	2.52617100	-0.03723300
C	1.08553700	1.04429300	0.03131700
C	2.39417800	0.54515600	0.04911200
C	4.85766000	0.33180300	-0.06780500
C	4.19619000	-0.88560600	0.09784200
N	2.81272900	-0.72827000	0.18830300
C	1.91521100	-1.83961500	0.46933300
H	1.16265900	-1.51500100	1.18044800
H	1.41961300	-2.17236600	-0.44145500
H	2.49471500	-2.65100100	0.89543800
C	-2.39417800	0.54515000	-0.04906900
C	-4.19618900	-0.88561500	-0.09784800
C	-4.85766400	0.33179800	0.06775200
N	-2.81272300	-0.72828100	-0.18824500
C	-1.91517500	-1.83962600	-0.46918200
H	-1.41951100	-2.17223100	0.44162200
H	-2.49466700	-2.65109400	-0.89514400
H	-1.16267500	-1.51507600	-1.18038300
N	0.00000000	0.27784500	0.00003300
H	-1.22965600	3.08352000	-0.77843500
H	1.22964600	3.08352600	0.77849800
C	-6.24018500	0.39854400	0.16282200
C	-4.91830600	-2.07364900	-0.15375100
C	-6.29662400	-2.00446000	-0.05628700
C	-6.95479000	-0.78387900	0.09670900
H	-6.74133800	1.34792300	0.28774500
H	-8.03246700	-0.76095000	0.16992700
H	-6.87223800	-2.91825000	-0.09594300
H	-4.42889100	-3.03040500	-0.25652500
C	4.91830300	-2.07364400	0.15373100
C	6.24017800	0.39854200	-0.16293500
C	6.95478100	-0.78388400	-0.09683500
C	6.29661700	-2.00446100	0.05620600
H	4.42888400	-3.03039400	0.25653700
H	6.87223100	-2.91825200	0.09584800
H	8.03245500	-0.76095900	-0.17010000
H	6.74133000	1.34791600	-0.28789300
S	3.71769100	1.63941200	-0.13743900
S	-3.71769700	1.63940800	0.13741200
H	1.13188400	2.95903600	-0.97228000
H	-1.13189200	2.95903400	0.97234200

Compound 4e (Singlet)

Absolute Energy = -287.751107 a.u.

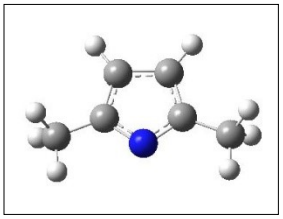


1 1

C	1.05779700	0.14978700	-0.00007100
C	0.66090700	-1.31458300	0.00005600
C	-0.66092200	-1.31457700	0.00003100
C	-1.05780000	0.14977300	-0.00006400
N	0.00000500	0.95598400	-0.00011300
H	1.35671000	-2.13862900	0.00012700
H	-1.35672800	-2.13862100	0.00008200
C	2.42651700	0.62011000	-0.00001500
H	2.94135700	0.18012200	0.86583800
H	2.94206200	0.17906500	-0.86486800
H	2.49841500	1.70157000	-0.00053900
C	-2.42650800	0.62012300	-0.00002000
H	-2.49838500	1.70158400	-0.00081200
H	-2.94223200	0.17881000	-0.86461800
H	-2.94118800	0.18041500	0.86608200

Compound 4e (triplet)

Absolute Energy = -287.713633 a.u.

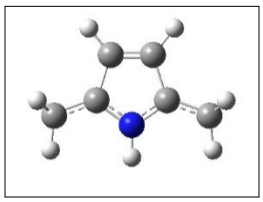


1 3

C	-1.10303300	-0.09404700	-0.00003500
C	-0.72288700	1.27784900	-0.00001300
C	0.72288700	1.27784900	-0.00002400
C	1.10303300	-0.09404700	-0.00003700
N	0.00000000	-0.88226600	-0.00008400
H	-1.37377100	2.13896200	-0.00001700
H	1.37377100	2.13896200	-0.00003900
C	-2.46789700	-0.64301000	0.00002800
H	-3.01472600	-0.28454700	0.87636800
H	-3.01536400	-0.28339700	-0.87542400
H	-2.44207700	-1.72783700	-0.00063000
C	2.46789700	-0.64301000	0.00005100
H	2.44207700	-1.72783700	-0.00097000
H	3.01553500	-0.28307900	-0.87515800
H	3.01455500	-0.28486600	0.87663400

Compound 4e (Protonated)

Absolute Energy = -287.911894 a.u.

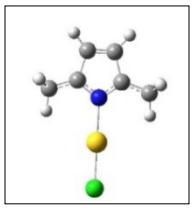


2 1

C	-1.11287800	-0.10233900	-0.00005100
C	-0.66628800	1.31880700	0.00008900
C	0.66629100	1.31880600	0.00008500
C	1.11287900	-0.10233500	-0.00008200
N	-0.00000200	-0.87971700	-0.00012500
H	-1.35157100	2.15562300	0.00017400
H	1.35157400	2.15562300	0.00016300
C	-2.45446500	-0.58823500	-0.00003500
H	-2.98112700	-0.11489800	0.85422200
H	-2.98178200	-0.11397100	-0.85331500
H	-2.56984400	-1.66774300	-0.00047100
C	2.45446300	-0.58823800	-0.00005400
H	2.56983800	-1.66774700	-0.00068700
H	2.98195200	-0.11375500	-0.85308900
H	2.98095900	-0.11512400	0.85444600
H	0.00000000	-1.89877600	-0.00027600

Compound 10 complex with AuCl

Absolute Energy = -883.312107 a.u.



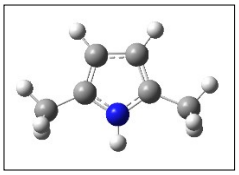
1 1

C	-2.13706100	-1.07462300	-0.00008300
C	-3.58628200	-0.66211800	0.00015000
C	-3.58642800	0.66164500	0.00017400
C	-2.13727500	1.07448700	-0.00006900
N	-1.33741400	0.00003500	-0.00019900
H	-4.41185500	-1.35653400	0.00025500
H	-4.41216000	1.35587300	0.00030500

C	-1.66612600	-2.43614200	-0.00002600
H	-2.11571800	-2.95009500	0.86434400
H	-2.11682200	-2.95079900	-0.86336200
H	-0.58349900	-2.52055500	-0.00057100
C	-1.66663600	2.43611300	-0.00006100
H	-0.58402400	2.52073200	-0.00096100
H	-2.11777400	2.95083200	-0.86311100
H	-2.11595300	2.94982600	0.86460500
Au	0.81784100	0.00007800	-0.00004800
Cl	3.05230100	-0.00010700	0.00018600

Compound 4e + Hydride ion

Absolute Energy = -288.678218 a.u.

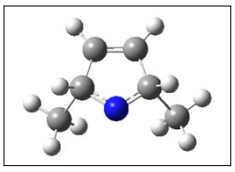


0 1

C	1.12895400	-0.02174000	-0.00004300
C	0.71228900	1.28208900	-0.00002600
C	-0.71222100	1.28210700	0.00002700
C	-1.12896100	-0.02177200	0.00003100
N	-0.00000500	-0.80208200	-0.00001100
H	1.36227600	2.14117400	0.00002300
H	-1.36215600	2.14123100	-0.00001800
C	2.49465900	-0.61639300	0.00002000
H	3.23793200	0.17777200	-0.00037300
H	2.66693000	-1.23574400	0.88264300
H	2.66671600	-1.23640500	-0.88217600
C	-2.49470900	-0.61634900	-0.00000700
H	-2.66707300	-1.23566400	-0.88263400
H	-2.66677100	-1.23638900	0.88217300
H	-3.23792300	0.17786800	0.00044900
H	0.00003700	-1.80691600	-0.00001200

Compound 4e (ASE)

Absolute Energy = - -288.996187 a.u.

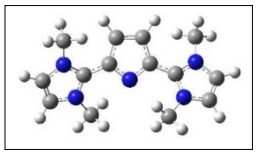


1 1

C	1.09022800	0.10344300	0.41831100
C	0.62629400	1.35369000	-0.23099700
C	-0.71240900	1.34601300	-0.20093300
C	-1.13238400	0.08426400	0.45685100
N	-0.00868200	-0.60061700	0.86974100
H	1.27083100	2.10199800	-0.66494600
H	-1.38548100	2.08423100	-0.60828300
H	-1.86156300	0.12247800	1.27859500
H	1.74585700	0.20465900	1.30498000
C	-1.88720100	-0.95918800	-0.52191600
H	-2.13044000	-1.85328900	0.03975500
H	-2.77958800	-0.43063000	-0.84333900
H	-1.24670400	-1.18022600	-1.36832500
C	1.99337100	-0.87209300	-0.46411800
H	2.82403800	-0.25531400	-0.79673800
H	2.33176800	-1.70235500	0.14434900
H	1.42466300	-1.22400000	-1.31742400

Compound 4f (Singlet)

Absolute Energy = -817.577542 a.u.



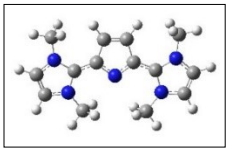
1 1

C	1.06860100	-0.58215700	-0.03161100
C	0.69108200	-1.94260800	-0.01690700
C	-0.69108200	-1.94260800	0.01690000
C	-1.06860200	-0.58215700	0.03161000
C	-2.39750900	-0.03180600	0.09435100
C	-4.59411900	0.23482700	-0.12013600
C	-4.10395400	1.33379200	0.48945500
H	-5.59663800	-0.02682800	-0.40463300
H	-4.59527200	2.22069200	0.84503500
N	-2.74525400	1.15528600	0.62182100
N	-3.52738300	-0.60070700	-0.36590700
C	-1.85154000	2.10544400	1.27258100
H	-1.14550200	1.56344300	1.89340800
H	-1.29857300	2.67015500	0.52729800
H	-2.45986100	2.76989400	1.87947500
C	-3.62659500	-1.87591000	-1.06072300
H	-3.67715500	-2.69666400	-0.34811800
H	-4.53001300	-1.86365900	-1.66323700
H	-2.75860700	-2.00109400	-1.70256100
C	2.39750900	-0.03180600	-0.09435000
C	4.10395500	1.33379100	-0.48945400
C	4.59411900	0.23482600	0.12013900
H	4.59527400	2.22069000	-0.84503500
H	5.59663700	-0.02682900	0.40463800
N	3.52738200	-0.60070700	0.36591000
N	2.74525500	1.15528500	-0.62182200

C	3.62659300	-1.87590900	1.06072800
H	2.75860000	-2.00109600	1.70255700
H	3.67716300	-2.69666300	0.34812400
H	4.53000500	-1.86365400	1.66325000
C	1.85154200	2.10544100	-1.27258400
H	1.29857600	2.67015500	-0.52730300
H	2.45986300	2.76989000	-1.87948000
H	1.14550300	1.56343900	-1.89340900
N	0.00000000	0.24048100	0.00000000
H	1.32888200	-2.80914300	-0.05582300
H	-1.32888200	-2.80914400	0.05581300

Compound 4f (Triplet)

Absolute Energy = -817.477179 a.u.

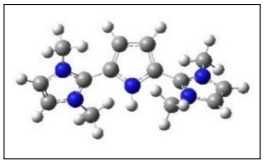


1 3

C	1.08972800	-0.55158800	0.00280100
C	0.66822700	-1.96705200	0.00286500
C	-0.66822600	-1.96705200	-0.00286600
C	-1.08972900	-0.55158800	-0.00280100
C	-2.38824700	-0.04838500	0.00986300
C	-4.62138300	0.14478100	-0.00510900
C	-4.10119300	1.39488700	0.05225300
H	-5.64573600	-0.17959600	-0.03123400
H	-4.59624500	2.34812100	0.08921500
N	-2.73997300	1.28953400	0.05959900
N	-3.58440700	-0.74364000	-0.03160700
C	-1.84803400	2.43451600	0.14109200
H	-1.23126700	2.36706600	1.03313400
H	-1.19982400	2.47006900	-0.72955800
H	-2.46814100	3.32565300	0.18330300
C	-3.75628100	-2.17913300	-0.11778500
H	-3.35656300	-2.66793900	0.76924100
H	-4.82022100	-2.38554200	-0.18254500
H	-3.26703600	-2.56794000	-1.00931300
C	2.38824600	-0.04838500	-0.00986300
C	4.10119400	1.39488600	-0.05225300
C	4.62138300	0.14478000	0.00510900
H	4.59624600	2.34812000	-0.08921500
H	5.64573600	-0.17959800	0.03123400
N	3.58440600	-0.74364000	0.03160700
N	2.73997400	1.28953400	-0.05959900
C	3.75627900	-2.17913400	0.11778500
H	3.26703300	-2.56794000	1.00931300
H	3.35656100	-2.66794000	-0.76924100
H	4.82021900	-2.38554400	0.18254600
C	1.84803600	2.43451700	-0.14109200
H	1.19982500	2.47007000	0.72955800
H	2.46814300	3.32565300	-0.18330300
H	1.23126800	2.36706700	-1.03313400
N	0.00000000	0.26917600	0.00000000
H	1.29273300	-2.84140900	0.00235300
H	-1.29273200	-2.84141000	-0.00235300

Compound 4f (Protonated)

Absolute Energy = -817.852413 a.u.



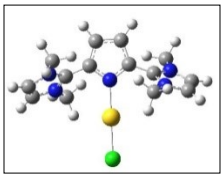
2 1

C	-1.11547200	0.03920500	0.52578600
C	-0.70343200	0.02345400	1.84019000
C	0.70343200	-0.02345700	1.84019000
C	1.11547200	-0.03920600	0.52578600
C	2.47138500	-0.09353100	0.00059600
C	4.61744000	0.32936400	-0.30088000
C	4.28810600	-0.72122700	-1.08992500
H	5.55597100	0.83550700	-0.15872200
H	4.88403500	-1.30862100	-1.76596700
N	2.95550000	-0.97583400	-0.88674300
N	3.48018800	0.70966400	0.36466700
C	2.21773100	-2.07502100	-1.50807300
H	1.40370200	-2.37146000	-0.85257700
H	1.83622600	-1.77145200	-2.48086000
H	2.89546300	-2.91396500	-1.63503500
C	3.41955100	1.81266600	1.32648500
H	3.71459700	1.45932400	2.31174000
H	4.10252700	2.58943400	0.99610300
H	2.40745600	2.20328300	1.35919900
C	-2.47138500	0.09353100	0.00059600
C	-4.28810600	0.72122800	-1.08992400
C	-4.61744000	-0.32936400	-0.30088000
H	-4.88403500	1.30862400	-1.76596500
H	-5.55597100	-0.83550700	-0.15872400
N	-3.48018800	-0.70966500	0.36466500
N	-2.95550000	0.97583500	-0.88674100
C	-3.41955100	-1.81266800	1.32648200
H	-2.40745600	-2.20328600	1.35919500
H	-3.71459700	-1.45932800	2.31173700
H	-4.10252700	-2.58943600	0.99609900

C	-2.21773000	2.07502400	-1.50807000
H	-1.83622600	1.77145600	-2.48085700
H	-2.89546300	2.91396800	-1.63503000
H	-1.40370200	2.37146200	-0.85257300
N	0.00000000	0.00000000	-0.27118400
H	-1.34585500	0.05972300	2.70414500
H	1.34585500	-0.05972800	2.70414500
H	0.00000000	0.00000100	-1.27886000

Compound 4f complex with AuCl

Absolute Energy = -1413.169538 a.u.

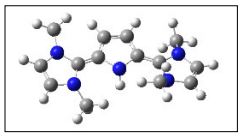


1 1

C	1.09681900	-1.68970100	-0.04321500
C	0.70155600	-3.03641800	-0.02333300
C	-0.70172300	-3.03638400	0.02254700
C	-1.09691700	-1.68965100	0.04303800
C	-2.45126000	-1.14984800	0.09935300
C	-4.55810200	-0.64722400	-0.44352900
C	-4.30262700	-0.10754100	0.78058200
H	-5.44915700	-0.62620800	-1.05231100
H	-4.92786600	0.47680600	1.43836900
N	-3.00292700	-0.43547000	1.10917200
N	-3.40471300	-1.28682900	-0.85474100
C	-2.34555400	-0.05993600	2.36737800
H	-1.50056500	-0.72736600	2.53419300
H	-1.98947700	0.97176600	2.30833600
H	-3.06659000	-0.16743300	3.18022200
C	-3.25083300	-1.96873600	-2.14452000
H	-3.81357200	-2.90594500	-2.14023800
H	-3.62397000	-1.31605700	-2.93671000
H	-2.19437400	-2.17873600	-2.30756400
C	2.45118400	-1.14991500	-0.09936000
C	4.30253500	-0.10743500	-0.78034900
C	4.55799200	-0.64733300	0.44367300
H	4.92776700	0.47706800	-1.43800300
H	5.44902200	-0.62638600	1.05249500
N	3.40463100	-1.28710400	0.85470500
N	3.00288100	-0.43541300	-1.10906500
C	3.25073100	-1.96917800	2.14439500
H	2.19444300	-2.18065100	2.30663000
H	3.81476900	-2.90560500	2.14051800
H	3.62236400	-1.31597900	2.93686900
C	2.34548000	-0.05966300	-2.36719100
H	1.98935800	0.97201100	-2.30791300
H	3.06650200	-0.16694700	-3.18007500
H	1.50052300	-0.72710200	-2.53413000
N	-0.00002100	-0.86757000	0.00007900
H	1.35257800	-3.90069100	-0.05838800
H	-1.35278900	-3.90063900	0.05722500
Au	0.00009400	1.20488600	0.00006700
Cl	-0.00006100	3.50956100	-0.00015900

Compound 4f + Hydride ion

Absolute Energy = -818.259149 a.u.



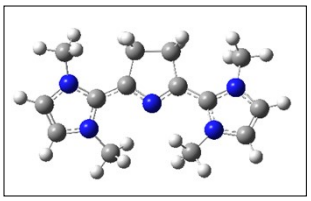
0 1

C	1.16265200	0.56885800	0.02287500
C	0.66711300	1.92333000	0.08165200
C	-0.68232100	1.91042000	0.01312700
C	-1.15636300	0.54894600	-0.09257000
C	-2.41872500	0.03966700	-0.04668300
C	-4.67383800	-0.17213800	0.09382700
C	-4.18114300	-1.39321900	-0.12615400
H	-5.68711600	0.15228400	0.24726700
H	-4.68488100	-2.33709600	-0.22573000
N	-2.78469200	-1.30814300	-0.18301600
N	-3.61655500	0.72650300	0.14493900
C	-2.02540100	-2.25798700	-0.96607700
H	-1.77676900	-1.84453300	-1.94979400
H	-1.11195700	-2.55526600	-0.45676400
H	-2.63787500	-3.14466300	-1.11363100
C	-3.73110600	2.09470600	0.56348400
H	-3.47780200	2.78755300	-0.24163900
H	-4.75979400	2.27858500	0.86485700
H	-3.07363600	2.29117800	1.41321100
C	2.41833700	0.05930200	0.07230200
C	4.14003300	-1.41470000	0.04801100
C	4.65561800	-0.19689600	-0.12320700
H	4.63012600	-2.37006900	0.10445200
H	5.67450300	0.10627500	-0.28811500
N	3.63061200	0.74499700	-0.07180900
N	2.73964000	-1.31281800	0.16213900
C	3.72735800	2.06973500	-0.61997700
H	3.03807100	2.18313600	-1.46261400
H	3.49098500	2.83408000	0.12210900
H	4.74514500	2.23459300	-0.96695100
C	2.08213600	-2.13736200	1.16547500
H	1.00455000	-2.07639400	1.04508800

H	2.40957200	-3.16772600	1.03522100
H	2.33696700	-1.80774000	2.17836400
N	0.01641300	-0.29800800	-0.07715700
H	1.27030700	2.80721600	0.20193600
H	-1.29894800	2.79117200	0.04814600
H	0.10452200	-0.88627500	-0.89759200

Compound 4f (ASE)

Absolute Energy = -818.729284 a.u.

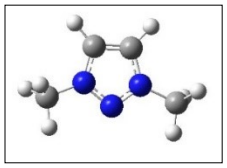


1 1

C	1.09374800	-0.59226700	0.00249700
C	0.77056000	-2.07815200	0.06807200
C	-0.77055700	-2.07815600	-0.06807600
C	-1.09375200	-0.59227200	-0.00250600
C	-2.37719600	-0.00200200	0.06743600
C	-4.59242500	0.30283700	-0.01666600
C	-4.03903500	1.45986700	0.38660800
H	-5.61894200	0.03489800	-0.18522600
H	-4.48789300	2.39994100	0.64898900
N	-2.67348100	1.26778200	0.44561100
N	-3.56564400	-0.59993400	-0.21130200
C	-1.73484100	2.27265900	0.90975300
H	-1.05419200	1.83123000	1.63261500
H	-1.15441800	2.66573700	0.07835200
H	-2.30600300	3.07158000	1.37389600
C	-3.75623900	-1.91715600	-0.79777500
H	-3.38874400	-2.69688500	-0.13730800
H	-4.82127000	-2.06139500	-0.95113600
H	-3.24996500	-1.97785200	-1.75892300
C	2.37719300	-0.00199900	-0.06743700
C	4.03904900	1.45985500	-0.38658800
C	4.59242400	0.30281700	0.01668600
H	4.48792000	2.39992500	-0.64896000
H	5.61893600	0.03486600	0.18525500
N	3.56563100	-0.59994500	0.21130400
N	2.67349400	1.26778300	-0.44561000
C	3.75620100	-1.91717600	0.79776500
H	3.24991600	-1.97787300	1.75890700
H	3.38869900	-2.69689100	0.13728600
H	4.82122800	-2.06143400	0.95113400
C	1.73487300	2.27267200	-0.90976600
H	1.15444200	2.66575600	-0.07837300
H	2.30605300	3.07158600	-1.37389900
H	1.05422900	1.83125200	-1.63263900
N	-0.00000400	0.15946900	-0.00000100
H	1.24306900	-2.64744100	-0.73123300
H	-1.24306200	-2.64744500	0.73123200
H	-1.07411400	-2.52740100	-1.01377000
H	1.07412200	-2.52739100	1.01376800

Compound 5 (Singlet)

Absolute Energy = -321.106550 a.u.

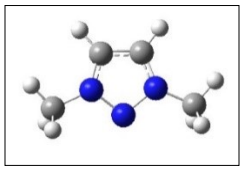


1 1

C	-0.68232500	-1.24347100	0.00066400
C	0.68232500	-1.24347100	-0.00056800
N	-1.03436700	0.06258700	0.00104600
N	0.00000000	0.85089400	-0.00009900
N	1.03436700	0.06258800	-0.00114800
C	2.38442500	0.63037300	0.00085000
H	2.89629700	0.31676800	0.90634800
H	2.91439900	0.27782000	-0.87942600
H	2.28224100	1.70972900	-0.02359700
C	-2.38442600	0.63037100	-0.00078000
H	-2.89742400	0.31425800	-0.90475900
H	-2.91330900	0.28028200	0.88114100
H	-2.28219800	1.70979000	0.02054900
H	-1.40275600	-2.04197300	0.00117100
H	1.40275700	-2.04197100	-0.00101200

Compound 5 (triplet)

Absolute Energy = -320.966577 a.u.



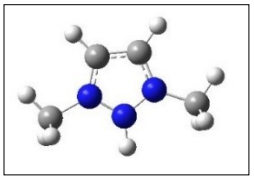
1 3

C	-0.70075900	-1.21602600	0.02881000
C	0.70197800	-1.21774400	0.03624400
N	-1.10726800	0.04638200	-0.17708900
N	-0.00405600	0.89148800	0.12477000

N	1.10987200	0.03894100	-0.14740100
C	2.43238900	0.61569300	0.02226500
H	2.54054800	1.00347400	1.03511200
H	3.16526900	-0.16376000	-0.16521500
H	2.55751700	1.41984700	-0.69775800
C	-2.43156300	0.61204100	0.03223900
H	-2.56262000	1.44928700	-0.64713300
H	-3.16331600	-0.15877300	-0.19208500
H	-2.53738300	0.94791200	1.06361700
H	-1.37891600	-2.04694500	0.14177400
H	1.37679500	-2.05249900	0.14238400

Compound 5 (Protonated)

Absolute Energy = -321.227232 a.u.

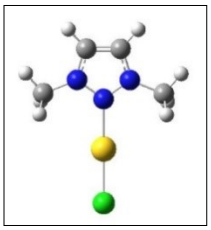


2 1

C	-0.69963800	-1.25186300	0.00006400
C	0.69964000	-1.25186200	0.00000100
N	-1.07580300	0.01949700	0.00011500
N	-0.00000100	0.77751800	-0.00016200
N	1.07580200	0.01949700	-0.00001800
C	2.44138000	0.60670500	-0.00000600
H	2.55595800	1.20351200	0.90338600
H	3.13855300	-0.22627600	-0.00058500
H	2.55552900	1.20442400	-0.90283200
C	-2.44138000	0.60670700	-0.00006700
H	-2.55578100	1.20359000	-0.90342400
H	-3.13854400	-0.22628400	0.00032900
H	-2.55571400	1.20433300	0.90280400
H	-1.40763600	-2.06841000	0.00003300
H	1.40764000	-2.06840700	-0.00011400
H	-0.00000100	1.79981600	0.00090700

Compound 5 complex with AuCl

Absolute Energy = -916.655925 a.u.

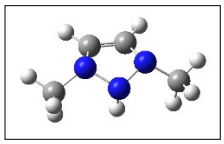


1 1

C	-3.40470500	-0.68840400	-0.00008500
C	-3.40443700	0.68910700	-0.00008000
N	-2.10132300	-1.06078900	0.00001000
N	-1.30098300	-0.00006300	0.00003500
N	-2.10091800	1.06100500	-0.00000900
C	-1.53328000	2.42230600	0.00005200
H	-2.36706500	3.12435300	-0.00008900
H	-0.92380300	2.55249100	0.89677800
H	-0.92352400	2.55243600	-0.89648700
C	-1.53413900	-2.42228400	0.00003900
H	-2.36813600	-3.12407900	0.00006600
H	-0.92458500	-2.55265000	-0.89660600
H	-0.92454100	-2.55260100	0.89665900
H	-4.21506600	-1.40267100	-0.00001300
H	-4.21453500	1.40367200	-0.00021300
Au	0.79315300	-0.00008900	0.00001700
Cl	3.05788900	0.00003900	-0.00007200

Compound 5 + Hydride ion

Absolute Energy = -321.859364 a.u.

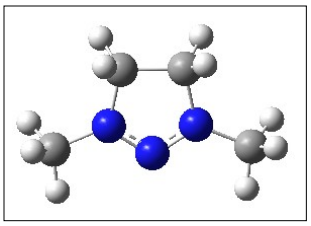


0 1

C	-0.66532600	1.23535500	-0.07609700
C	0.66541600	1.23553500	-0.07623700
N	-1.11233300	-0.02572600	0.38936700
N	-0.00001000	-0.90269000	0.15388400
N	1.11267500	-0.02570900	0.39047500
C	2.31392800	-0.57522100	-0.18922200
H	2.19543400	-0.76508300	-1.26734800
H	3.12993000	0.12925600	-0.04347100
H	2.55752100	-1.50924000	0.31211000
C	-2.31430700	-0.57508400	-0.18882800
H	-3.12959800	0.13013900	-0.04299800
H	-2.19683300	-0.76605900	-1.26687500
H	-2.55803700	-1.50848100	0.31358000
H	-1.35679500	2.04424500	-0.23794600
H	1.35685800	2.04466900	-0.23676300
H	0.00092400	-1.04407300	-0.88406700

Compound 5 (ASE)

Absolute Energy = -322.268002 a.u.

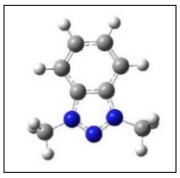


1 1

C	0.76729200	1.29155400	-0.00028800
C	-0.76729200	1.29155300	0.00029000
N	1.04680900	-0.15515400	0.00057300
N	0.00000000	-0.87218700	-0.00000500
N	-1.04680900	-0.15515400	-0.00058200
C	-2.37635300	-0.74147000	0.00004500
H	-2.91137800	-0.41645900	0.89082100
H	-2.91268200	-0.41526300	-0.88948800
H	-2.26987800	-1.82135800	-0.00076000
C	2.37635300	-0.74147000	-0.00003800
H	2.91137600	-0.41649900	-0.89083000
H	2.91268500	-0.41522300	0.88947900
H	2.26987900	-1.82135800	0.00081600
H	1.20418700	1.74499000	-0.88807600
H	-1.20419100	1.74498400	0.88808000
H	1.20488400	1.74632400	0.88644500
H	-1.20488000	1.74633100	-0.88644100

Compound 6 (Singlet)

Absolute Energy = -474.702104 a.u.

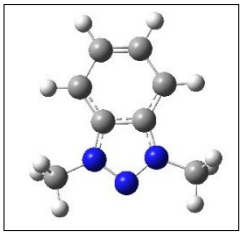


1 1

C	0.21396900	-0.69635300	0.00000000
C	0.21396900	0.69635300	0.00000000
C	1.39753500	1.44091400	0.00000000
C	2.55879200	0.70805900	0.00000000
C	2.55879200	-0.70805900	0.00000000
C	1.39753500	-1.44091400	0.00000000
H	1.39861700	2.52117800	0.00000000
H	3.50811900	1.22458600	0.00000000
H	3.50811900	-1.22458600	0.00000000
H	1.39861700	-2.52117800	0.00000000
N	-1.11084200	1.04370900	0.00000000
N	-1.88192400	0.00000000	0.00000000
N	-1.11084200	-1.04370900	0.00000000
C	-1.68305700	2.38532000	0.00000000
H	-1.35240100	2.91099400	0.89240700
H	-1.35240000	2.91099500	-0.89240600
H	-2.76273500	2.28277900	-0.00000100
C	-1.68305700	-2.38532000	0.00000000
H	-1.35240100	-2.91099400	-0.89240600
H	-1.35240100	-2.91099500	0.89240600
H	-2.76273500	-2.28277900	0.00000000

Compound 6 (triplet)

Absolute Energy = -474.594663 a.u.

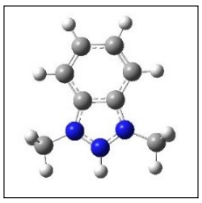


1 3

C	0.17863500	-0.70069000	0.00000000
C	0.17863500	0.70069000	0.00000000
C	1.38088700	1.43774700	0.00000000
C	2.62624900	0.67173500	0.00000000
C	2.62624900	-0.67173500	0.00000000
C	1.38088700	-1.43774700	0.00000000
H	1.38893200	2.51702800	0.00000000
H	3.55615800	1.22062100	0.00000000
H	3.55615800	-1.22062100	0.00000000
H	1.38893200	-2.51702800	0.00000000
N	-1.11126400	1.05719000	0.00000000
N	-1.94988000	0.00000000	0.00000000
N	-1.11126400	-1.05719000	0.00000000
C	-1.67000500	2.39941900	0.00000000
H	-1.34303900	2.92852500	0.89282000
H	-1.34303800	2.92852600	-0.89281900
H	-2.75018300	2.30139700	-0.00000100
C	-1.67000500	-2.39941900	0.00000000
H	-1.34303800	-2.92852500	-0.89281900
H	-1.34303800	-2.92852500	0.89281900
H	-2.75018300	-2.30139700	0.00000000

Compound 6 (Protonated)

Absolute Energy = -474.844158 a.u.

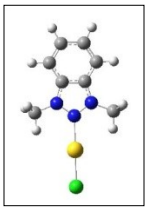


2 1

C	0.23380800	-0.71122400	0.00000000
C	0.23380800	0.71122400	0.00000000
C	1.42307800	1.45934300	0.00000000
C	2.56960900	0.71720200	0.00000000
C	2.56960900	-0.71720200	0.00000000
C	1.42307800	-1.45934300	0.00000000
H	1.42823800	2.54009700	0.00000000
H	3.52531400	1.22484100	0.00000000
H	3.52531400	-1.22484100	0.00000000
H	1.42823800	-2.54009700	0.00000000
N	-1.06042900	1.08256800	0.00000000
N	-1.80384800	0.00000000	0.00000000
N	-1.06042900	-1.08256800	0.00000000
C	-1.64032500	2.44042800	0.00000000
H	-1.29902400	2.95055700	0.89844700
H	-1.29902200	2.95055700	-0.89844600
H	-2.72429000	2.36034700	-0.00000100
C	-1.64032500	-2.44042800	0.00000000
H	-1.29902300	-2.95055700	-0.89844700
H	-1.29902300	-2.95055700	0.89844600
H	-2.72429000	-2.36034700	0.00000000
H	-2.82352000	0.00000000	0.00000000

Compound 6 complex with AuCl

Absolute Energy = -1070.252126 a.u.

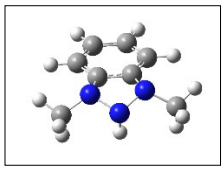


1 1

C	0.00000000	0.70422900	-2.62278100
C	0.00000000	-0.70422900	-2.62278100
C	0.00000000	-1.44983300	-3.81324300
C	0.00000000	-0.71163000	-4.98539600
C	0.00000000	0.71163000	-4.98539600
C	0.00000000	1.44983300	-3.81324300
H	0.00000000	-2.53429600	-3.81743900
H	0.00000000	-1.23241000	-5.93779200
H	0.00000000	1.23241000	-5.93779200
H	0.00000000	2.53429600	-3.81743900
N	0.00000000	-1.07026700	-1.30023900
N	0.00000000	0.00000000	-0.51291400
N	0.00000000	1.07026700	-1.30023900
C	0.00000000	-2.43487700	-0.75420100
H	-0.89882400	-2.95125000	-1.09978300
H	0.89882200	-2.95125100	-1.09978500
H	0.00000100	-2.37410700	0.33476600
C	0.00000000	2.43487700	-0.75420100
H	0.89882400	2.95125000	-1.09978300
H	-0.89882200	2.95125100	-1.09978500
H	-0.00000100	2.37410700	0.33476600
Au	0.00000000	0.00000000	1.58949000
Cl	0.00000000	0.00000000	3.85714800

Compound 6 + Hydride ion

Absolute Energy = -475.471745 a.u.

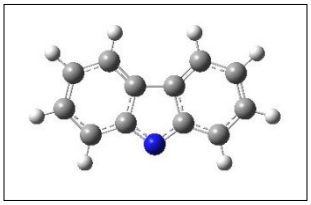


0 1

C	-0.21291900	0.69914700	0.16771800
C	-0.21299500	-0.69912500	0.16776000
C	-1.38174400	-1.41397300	0.02905000
C	-2.57307900	-0.69199900	-0.10463900
C	-2.57300500	0.69225300	-0.10468200
C	-1.38159200	1.41411200	0.02894100
H	-1.38470700	-2.49529400	0.02396600
H	-3.50544800	-1.22728300	-0.21871200
H	-3.50531500	1.22763000	-0.21880200
H	-1.38443500	2.49543200	0.02379000
N	1.11392000	-1.11335900	0.38128400
N	1.92294000	-0.00008300	-0.03464900
N	1.11401400	1.11323200	0.38121800
C	1.56485900	-2.34494300	-0.21477600
H	0.95287800	-3.16239400	0.15944400
H	1.49117100	-2.32095000	-1.31221400
H	2.59864200	-2.51930200	0.07377400
C	1.56518900	2.34478800	-0.21467000
H	1.49176600	2.32084700	-1.31213400
H	0.95319300	3.16229500	0.15940600
H	2.59892200	2.51904900	0.07411600
H	1.86893000	-0.00012500	-1.07581900

Compound 7 (Singlet)

Absolute Energy = -516.371020 a.u.

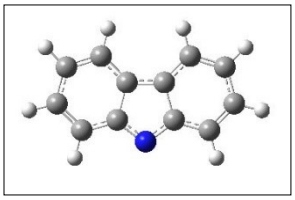


1 1

C	-3.07036200	1.04571100	-0.00012900
C	-3.41351700	-0.29543200	-0.00010800
C	-2.41548400	-1.26776800	-0.00002300
C	-1.08767900	-0.82839200	-0.00004600
C	-0.74070000	0.55803700	-0.00008200
C	-1.71717100	1.49907600	-0.00009200
H	-3.85847800	1.78745800	-0.00013800
H	-4.45419300	-0.58374900	-0.00013800
H	-2.63750200	-2.32654900	-0.00005000
H	-1.50681700	2.55958200	-0.00007200
C	1.08767900	-0.82839200	0.00004600
C	2.41548400	-1.26776800	0.00018000
C	3.41351700	-0.29543200	0.00017900
C	3.07036200	1.04571100	0.00012900
C	1.71717100	1.49907600	0.00005200
C	0.74070000	0.55803700	-0.00002000
H	2.63750100	-2.32654900	0.00017200
H	4.45419300	-0.58374900	0.00023600
H	3.85847900	1.78745800	0.00018600
H	1.50681700	2.55958200	0.00005200
N	0.00000000	-1.62975300	-0.00011000

Compound 7 (triplet)

Absolute Energy = -516.356856 a.u.

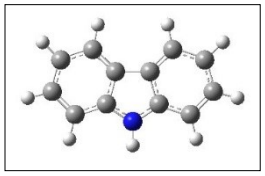


1 3

C	-3.00601400	1.10971400	-0.00013800
C	-3.36500900	-0.27045100	-0.00013900
C	-2.42035400	-1.27255900	-0.00008800
C	-1.07847200	-0.88206700	-0.00003500
C	-0.71063700	0.52819900	-0.00003500
C	-1.68722000	1.51893300	-0.00008700
H	-3.79724500	1.84655200	-0.00018000
H	-4.41615400	-0.52532900	-0.00018000
H	-2.68591200	-2.31989500	-0.00008900
H	-1.43023600	2.56901900	-0.00008600
C	1.07847200	-0.88206700	0.00005500
C	2.42035400	-1.27255900	0.00011400
C	3.36500900	-0.27045100	0.00014300
C	3.00601400	1.10971400	0.00011400
C	1.68722000	1.51893300	0.00005600
C	0.71063700	0.52819900	0.00002500
H	2.68591200	-2.31989500	0.00013500
H	4.41615400	-0.52532900	0.00019000
H	3.79724500	1.84655200	0.00014000
H	1.43023600	2.56901900	0.00003500
N	0.00000000	-1.70313100	0.00001700

Compound 7 (Protonated)

Absolute Energy = -516.555801 a.u.

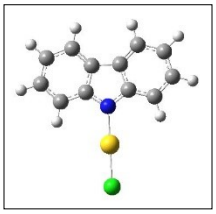


2 1

C	-3.07920300	1.07649800	-0.00012300
C	-3.44260800	-0.26877600	-0.00014200
C	-2.46606400	-1.24741500	-0.00010800
C	-1.12319200	-0.80144000	-0.00005400
C	-0.73936300	0.57525900	-0.00003200
C	-1.71053700	1.52144200	-0.00006700
H	-3.85811100	1.83008500	-0.00015200
H	-4.48793000	-0.54372300	-0.00018200
H	-2.71331400	-2.30241200	-0.00011900
H	-1.49720300	2.58205000	-0.00005700
C	1.12319200	-0.80144000	0.00004100
C	2.46606400	-1.24741500	0.00009900
C	3.44260800	-0.26877600	0.00014700
C	3.07920300	1.07649800	0.00013500
C	1.71053700	1.52144300	0.00007600
C	0.73936300	0.57525900	0.00003000
H	2.71331400	-2.30241200	0.00010800
H	4.48793000	-0.54372300	0.00019500
H	3.85811100	1.83008500	0.00017300
H	1.49720300	2.58205000	0.00006800
N	0.00000000	-1.54706900	-0.00000500
H	0.00000000	-2.56934400	-0.00001400

Compound 7 complex with AuCl

Absolute Energy = -1111.947762 a.u.

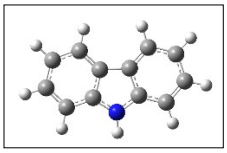


1 1

C	3.18634400	3.05850600	-0.00067700
C	1.84678100	3.41927000	-0.00061300
C	0.85990300	2.44047200	-0.00047400
C	1.28182600	1.10800400	-0.00034000
C	2.65325100	0.73722100	-0.00041500
C	3.61195900	1.70308700	-0.00058500
H	3.93919600	3.83570300	-0.00080800
H	1.57090400	4.46338700	-0.00066800
H	-0.19427500	2.68883300	-0.00039500
H	4.66738600	1.46898800	-0.00067300
C	1.28133600	-1.10815500	-0.00020200
C	0.85884300	-2.44045100	-0.00018300
C	1.84530200	-3.41967000	-0.00019400
C	3.18502000	-3.05948100	-0.00028700
C	3.61122100	-1.70424800	-0.00036400
C	2.65293100	-0.73796600	-0.00032100
H	-0.19543700	-2.68837100	-0.00009900
H	1.56898200	-4.46367000	-0.00013300
H	3.93753400	-3.83700600	-0.00032400
H	4.66675000	-1.47061300	-0.00047900
N	0.48139900	0.00010500	-0.00007000
Au	-1.52910100	0.00032400	0.00038700
Cl	-3.75177600	-0.00018400	0.00008300

Compound 7 + Hydride ion

Absolute Energy = -517.302118 a.u.

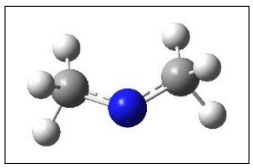


0 1

C	3.04784100	1.11312000	-0.00035000
C	3.42174300	-0.22912800	-0.00051700
C	2.46446200	-1.23048300	-0.00013600
C	1.12861800	-0.82538300	0.00029100
C	0.73263700	0.53453200	0.00053300
C	1.69698900	1.50959300	0.00022700
H	3.81620200	1.87367200	-0.00072500
H	4.46957900	-0.49129800	-0.00093200
H	2.73898800	-2.27655000	-0.00010000
H	1.43990900	2.55976000	0.00039600
C	-1.12867200	-0.82538300	0.00028900
C	-2.46475600	-1.23038300	-0.00012700
C	-3.42177400	-0.22903900	-0.00051100
C	-3.04759200	1.11331900	-0.00035400
C	-1.69674900	1.50973700	0.00021600
C	-0.73245900	0.53464300	0.00049700
H	-2.73933900	-2.27643000	-0.00011100
H	-4.46968000	-0.49092600	-0.00092200
H	-3.81591800	1.87391500	-0.00071300
H	-1.43966200	2.55989900	0.00041700
N	-0.00022600	-1.59882300	0.00031300
H	-0.00021400	-2.61115500	0.00014800

Compound 8a (Singlet)

Absolute Energy = -134.105527 a.u.

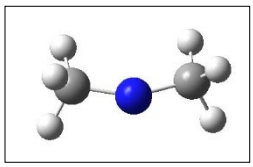


1 1

C	-1.18663200	-0.17759100	-0.00022300
C	1.18664500	-0.17757900	0.00019200
N	-0.00000700	0.50241900	0.00000300
H	1.77966800	0.28617400	0.82170400
H	1.17134700	-1.26458400	0.00048500
H	-1.17134700	-1.26459700	-0.00070700
H	-1.77837400	0.28528700	0.82285900
H	1.77852000	0.28544400	-0.82269000
H	-1.77984400	0.28636200	-0.82148100

Compound 8a (triplet)

Absolute Energy = -134.110503 a.u.



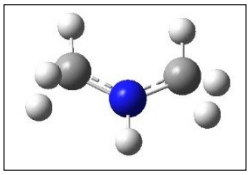
1 3

C	-1.35167900	-0.07663800	0.00013000
C	1.35167900	-0.07663900	-0.00012700
N	0.00000000	0.27455000	-0.00000400

H	1.83274300	0.33635400	0.89411800
H	1.42808400	-1.17208800	0.00090000
H	-1.42808400	-1.17208700	-0.00114300
H	-1.83208800	0.33443700	0.89561800
H	1.83214700	0.33464000	-0.89548900
H	-1.83280100	0.33655800	-0.89398900

Compound 8a (Protonated)

Absolute Energy = -134.168203 a.u.

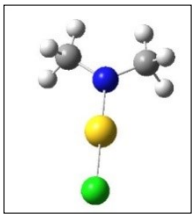


2 1

C	-1.21496700	-0.22247000	-0.00011100
C	1.21497500	-0.22246300	0.00007000
N	-0.00000200	0.38245000	0.00001500
H	1.86250500	0.29683600	0.78871200
H	1.22861100	-1.30919400	0.00014100
H	-1.22860800	-1.30920100	-0.00035600
H	-1.86172500	0.29618300	0.78981000
H	1.86178300	0.29633500	-0.78969100
H	-1.86258900	0.29699900	-0.78855700
H	-0.00000400	1.42448800	0.00007800

Compound 8a complex with AuCl

Absolute Energy = -729.678470 a.u.

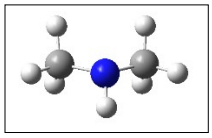


1 1

C	2.49042300	-1.22892500	0.00003200
C	2.49042100	1.22892600	0.00014800
N	1.74321100	0.00000000	0.00005300
H	2.17690700	1.83117400	0.87123200
H	3.56997400	1.06985600	0.00102900
H	3.56997600	-1.06985400	-0.00110800
H	2.17862400	-1.82989900	0.87267700
H	2.17841000	1.83012400	-0.87225700
H	2.17669700	-1.83139900	-0.87081000
Au	-0.20655200	0.00000000	-0.00001300
Cl	-2.44826600	0.00000000	-0.00007100

Compound 8a + Hydride ion

Absolute Energy = -135.077021 a.u.

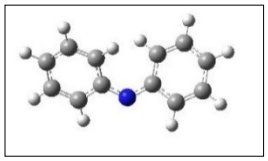


0 1

C	-1.20445600	0.22358000	0.02029000
C	1.20450200	0.22364000	0.02030200
N	-0.00003800	-0.56749500	-0.14817000
H	2.08286700	-0.41568900	-0.05430800
H	1.26087600	0.96351800	-0.77988800
H	-1.25844200	0.96645700	-0.77728800
H	-2.08323700	-0.41468700	-0.05876400
H	1.24534900	0.76457900	0.97688800
H	-1.24742400	0.76118200	0.97868100
H	0.00000500	-1.33620800	0.50831500

Compound 8b (Singlet)

Absolute Energy = -517.556711 a.u.



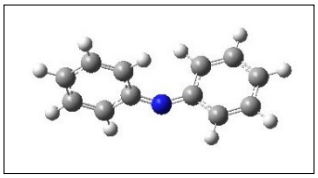
1 1

N	0.00000000	-1.08279200	0.00000000
C	-1.18315700	-0.46667200	0.05749400
C	-2.29902300	-1.26093600	-0.33452700
C	-1.40118000	0.86342100	0.52820800
C	-3.55361000	-0.70676000	-0.38451800
H	-2.10681700	-2.28203300	-0.63354900
C	-2.66940300	1.38283000	0.51741100
H	-0.58452200	1.41157100	0.97647800
C	-3.73637000	0.61141000	0.03873700
H	-4.39807100	-1.28949900	-0.72276600
H	-2.85627300	2.37416900	0.90477800
H	-4.73202700	1.03580300	0.03533900
C	1.18315700	-0.46667100	-0.05749300
C	1.40118000	0.86342000	-0.52820900
C	2.29902300	-1.26093600	0.33452700

C	2.66940300	1.38283000	-0.51741100
H	0.58452100	1.41157100	-0.97647800
C	3.55361000	-0.70676000	0.38451700
H	2.10681700	-2.28203400	0.63354800
C	3.73636900	0.61141000	-0.03873600
H	2.85627300	2.37416900	-0.90477800
H	4.39807100	-1.28949900	0.72276600
H	4.73202700	1.03580300	-0.03533900

Compound 8b (triplet)

Absolute Energy = -517.543526 a.u.

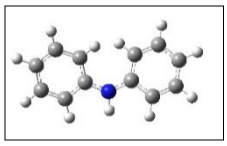


1 3

N	0.00000000	0.00000000	0.68357200
C	0.00000000	-1.25983800	0.31874100
C	0.78826400	-2.20895300	1.03867400
C	-0.83003700	-1.69512300	-0.76350100
C	0.75640300	-3.52583300	0.66798200
H	1.39263300	-1.85948800	1.86344700
C	-0.83072100	-3.01673000	-1.11493100
H	-1.43204500	-0.96284000	-1.28345900
C	-0.04559200	-3.93750800	-0.40507600
H	1.35105300	-4.25173400	1.20385800
H	-1.44215100	-3.35511200	-1.93948400
H	-0.06289800	-4.98070700	-0.68820300
C	0.00000000	1.25983800	0.31874100
C	0.83003700	1.69512300	-0.76350100
C	-0.78826400	2.20895300	1.03867400
C	0.83072100	3.01673000	-1.11493100
H	1.43204500	0.96284000	-1.28345900
C	-0.75640300	3.52583300	0.66798200
H	-1.39263300	1.85948800	1.86344700
C	0.04559200	3.93750800	-0.40507600
H	1.44215100	3.35511200	-1.93948400
H	-1.35105300	4.25173400	1.20385800
H	0.06289800	4.98070700	-0.68820300

Compound 8b (Protonated)

Absolute Energy = -517.743903 a.u.

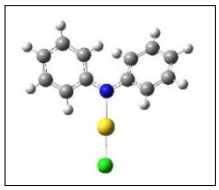


2 1

N	0.00000000	0.95029200	0.00000000
C	-1.23199500	0.40729800	-0.05366800
C	-2.32436800	1.27470800	0.27195000
C	-1.46623800	-0.94682900	-0.44889400
C	-3.58993200	0.76575100	0.31591100
H	-2.13011400	2.30921400	0.53202300
C	-2.74330900	-1.42652600	-0.41567800
H	-0.66215000	-1.54137500	-0.85893500
C	-3.80161700	-0.58442000	-0.01663100
H	-4.42541600	1.39282500	0.59432200
H	-2.95625600	-2.43550600	-0.74075400
H	-4.81132600	-0.97798400	-0.00725000
C	1.23199500	0.40729800	0.05366800
C	1.46623800	-0.94682900	0.44889400
C	2.32436800	1.27470800	-0.27195000
C	2.74330900	-1.42652600	0.41567800
H	0.66215000	-1.54137500	0.85893500
C	3.58993200	0.76575100	-0.31591100
H	2.13011400	2.30921400	-0.53202300
C	3.80161700	-0.58442000	0.01663100
H	2.95625600	-2.43550600	0.74075400
H	4.42541600	1.39282500	-0.59432200
H	4.81132600	-0.97798400	0.00725000
H	0.00000000	1.97382000	0.00000000

Compound 8b complex with AuCl

Absolute Energy = -1113.121961 a.u.



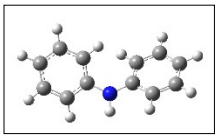
1 1

N	0.00000000	0.00000000	-0.68436400
C	0.27059300	1.14992500	-1.35775500
C	0.00000000	2.39299800	-0.72369900
C	0.88311700	1.13756800	-2.64353400
C	0.24695700	3.56405400	-1.39097000
H	-0.45453800	2.39504100	0.25858700
C	1.15657200	2.32353700	-3.27897000
H	1.22233900	0.19964500	-3.05997300

C	0.82518400	3.53292700	-2.66531700
H	0.00555200	4.51068400	-0.92950300
H	1.65971900	2.32195600	-4.23516800
H	1.04804500	4.46368900	-3.17026300
C	-0.27059300	-1.14992500	-1.35775500
C	-0.88311700	-1.13756800	-2.64353400
C	0.00000000	-2.39299800	-0.72369900
C	-1.15657200	-2.32353700	-3.27897000
H	-1.22233900	-0.19964500	-3.05997300
C	-0.24695700	-3.56405400	-1.39097000
H	0.45453800	-2.39504100	0.25858700
C	-0.82518400	-3.53292700	-2.66531700
H	-1.65971900	-2.32195600	-4.23516800
H	-0.00555200	-4.51068400	-0.92950300
H	-1.04804500	-4.46368900	-3.17026300
Au	0.00000000	0.00000000	1.39459200
Cl	0.00000000	0.00000000	3.62431700

Compound 8b + Hydride ion

Absolute Energy = -518.460803 a.u.

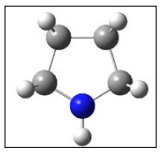


0 1

N	-0.00000400	-1.06366800	-0.00022700
C	1.25397900	-0.45769800	-0.02011100
C	2.35443800	-1.17705300	0.45367100
C	1.46251900	0.81948800	-0.54523600
C	3.62625700	-0.63326700	0.40659300
H	2.19980200	-2.16703100	0.86515600
C	2.73869400	1.35998200	-0.57210800
H	0.63083200	1.37519800	-0.95346000
C	3.82890600	0.64439000	-0.09769300
H	4.46321200	-1.20998300	0.77732800
H	2.88070400	2.35026300	-0.98440600
H	4.82076900	1.07278200	-0.12502700
C	-1.25402200	-0.45767200	0.01989600
C	-1.46239400	0.81957500	0.54496100
C	-2.35456600	-1.17705700	-0.45356900
C	-2.73854000	1.36007400	0.57209200
H	-0.63058100	1.37529100	0.95291400
C	-3.62638200	-0.63323500	-0.40624600
H	-2.20006800	-2.16708800	-0.86497800
C	-3.82888400	0.64444900	0.09797700
H	-2.88048100	2.35039000	0.98433100
H	-4.46342700	-1.20997300	-0.77674300
H	-4.82072100	1.07289000	0.12549700
H	-0.00004600	-2.06893600	-0.00039300

Pyrrolidine (Singlet)

Absolute Energy = -212.446592 a.u.

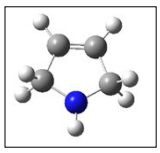


0 1

C	-1.22570000	-0.44344900	0.00010500
C	-0.77213800	1.02878500	-0.00003900
C	0.77213800	1.02878500	0.00020400
C	1.22570000	-0.44344900	-0.00006700
N	0.00000000	-1.19887100	-0.00024700
H	-1.15923000	1.54779200	0.87418800
H	1.15922500	1.54786400	-0.87398300
H	1.84219100	-0.65566700	-0.88036700
H	0.00000000	-2.19927300	-0.00026500
H	-1.84240200	-0.65583200	-0.88000600
H	-1.84193700	-0.65581700	0.88055000
H	-1.15894600	1.54752600	-0.87455000
H	1.15895100	1.54745400	0.87475500
H	1.84214800	-0.65598300	0.88018900

2,5-dihydro-1H-pyrrole (Singlet)

Absolute Energy = -211.251671 a.u.

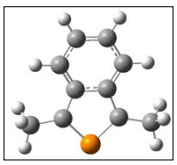


0 1

C	-1.21163700	0.35176700	0.00001100
C	-0.66199300	-1.04747100	-0.00007800
C	0.66199200	-1.04747100	-0.00007100
C	1.21163700	0.35176700	0.00002400
N	0.00000000	1.13618200	0.00010700
H	1.84192000	0.52604200	0.88242600
H	0.00000000	2.13520200	0.00014800
H	-1.84192900	0.52604200	0.88240600
H	-1.84188000	0.52616800	-0.88239400
H	1.84189000	0.52616800	-0.88237500
H	-1.29578500	-1.92222300	-0.00014500
H	1.29578500	-1.92222300	-0.00013100

Compound XVI′ (Singlet)

Absolute Energy = -727.965932 a.u.

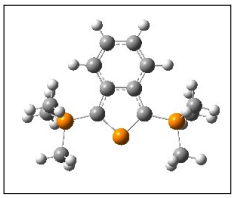


1 1

C	-0.97134300	1.23362500	0.00035000
C	0.39203300	0.70553600	0.00026200
C	0.39311700	-0.70516200	0.00020300
C	-0.96858300	-1.23511000	0.00030800
C	-1.24579200	-2.68001000	0.00005600
C	-1.24960200	2.67847200	0.00003000
P	-2.22164200	-0.00110300	-0.00005400
C	1.56969800	-1.40469500	0.00004900
C	1.56739500	1.40653300	0.00001100
C	2.79294700	-0.68251400	-0.00011300
C	2.79179600	0.68582000	-0.00011700
H	3.72779400	-1.22478000	-0.00051400
H	3.72585600	1.22948000	0.00002200
H	1.58415200	-2.48705200	0.00053000
H	1.58050700	2.48889800	-0.00030700
H	-0.78300300	3.13965900	-0.87763600
H	-2.31133100	2.90560600	0.00486400
H	-0.77345300	3.14293300	0.87060600
H	-0.77172300	-3.14438900	0.87168500
H	-2.30740700	-2.90795100	0.00190000
H	-0.77675100	-3.14082700	-0.87657200

Compound XVI″ (Singlet)

Absolute Energy = -1570.295246 a.u.

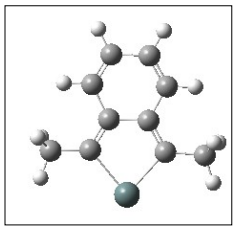


0 1

C	-1.27327800	0.35200300	0.00063100
C	-0.71465000	-0.98657000	0.00030700
C	0.71463000	-0.98657600	0.00010100
C	1.27327100	0.35199500	0.00014000
C	1.38701900	-2.21499600	-0.00001200
C	-1.38706000	-2.21497900	0.00027300
C	0.69569900	-3.41682800	-0.00005800
C	-0.69575500	-3.41681900	0.00006400
H	1.23906900	-4.35259800	-0.00015700
H	-1.23913600	-4.35258300	0.00004300
H	2.47121700	-2.24363100	-0.00001800
H	-2.47126000	-2.24360100	0.00047900
Si	0.00000500	1.68440700	0.00057100
P	-2.93971200	0.66131500	-0.00006900
P	2.93971400	0.66130200	-0.00006800
C	-3.85394700	0.01760600	-1.43330100
H	-3.68683800	-1.05416100	-1.52231800
H	-4.92192500	0.21476100	-1.34197000
H	-3.46370800	0.50078700	-2.32778200
C	-3.85536800	0.01746100	1.43220300
H	-4.92320100	0.21497600	1.33993300
H	-3.68870400	-1.05438000	1.52113100
H	-3.46582100	0.50031500	2.32716300
C	-3.28712200	2.43117900	-0.00004400
H	-2.84337000	2.88789600	0.88232800
H	-2.84394900	2.88787100	-0.88271500
H	-4.36525100	2.58854500	0.00030300
C	3.28707600	2.43117700	-0.00048200
H	2.84379500	2.88804900	0.88204400
H	4.36519700	2.58858800	-0.00075900
H	2.84338600	2.88768300	-0.88299300
C	3.85466900	0.01727700	-1.43270300
H	4.92241800	0.21568400	-1.34134200
H	3.68880000	-1.05474100	-1.52090300
H	3.46407100	0.49933500	-2.32763300
C	3.85476200	0.01778700	1.43273500
H	3.68834900	-1.05411300	1.52150700
H	4.92259600	0.21560200	1.34112900
H	3.46449700	0.50048400	2.32746400

Compound XVII′ (Singlet)

Absolute Energy = -601.085589 a.u.



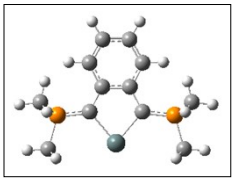
0 1

C	-0.13793500	-1.43001500	0.07490900
C	1.03200700	-0.75430700	0.02703700
C	1.03154600	0.75424400	0.02506300
C	-0.13838900	1.42951000	0.08013300
C	2.33175400	1.41895100	-0.01908100
C	2.33268200	-1.41844800	-0.01107900
C	3.48027800	0.72822900	-0.05206200
C	3.48079500	-0.72722100	-0.04732500
H	4.42926500	1.24755500	-0.08409200

H	4.43014800	-1.24608900	-0.07558800
H	2.35053900	2.50079400	-0.02433800
H	2.35209400	-2.50029200	-0.01030800
Sn	-1.80072400	-0.00006800	-0.03840100
C	-0.21680300	2.93138800	0.09185100
H	0.23213200	3.37047400	-0.80394600
H	-1.24618000	3.28458300	0.14110100
H	0.31014400	3.35324800	0.95226400
C	-0.21603600	-2.93185600	0.08820000
H	-1.24550300	-3.28529100	0.13365300
H	0.23643600	-3.37151400	-0.80552600
H	0.30773200	-3.35291700	0.95095600

Compound XVII″ (Singlet)

Absolute Energy = -1443.337896 a.u.

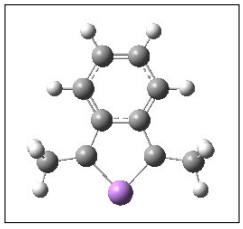


0 1

C	-1.37251800	-0.00719100	-0.00003400
C	-0.71809000	1.28774000	0.00003600
C	0.71809000	1.28773900	0.00007200
C	1.37251700	-0.00719100	0.00003700
C	1.37616000	2.52981400	0.00014700
C	-1.37615800	2.52981700	0.00009600
C	0.69528000	3.73451500	0.00018900
C	-0.69527500	3.73451700	0.00016900
H	1.24426800	4.66698800	0.00025100
H	-1.24426000	4.66699100	0.00021300
H	2.45957300	2.56122500	0.00018300
H	-2.45957000	2.56123200	0.00009400
P	-3.05043600	-0.19104900	-0.00006600
P	3.05043400	-0.19105300	0.00000600
C	-3.94232500	0.49497900	1.43334800
H	-3.71320800	1.55323600	1.53966700
H	-5.01925400	0.36333300	1.32860200
H	-3.59291000	-0.02189700	2.32598800
C	-3.94229100	0.49495400	-1.43351700
H	-5.01922200	0.36330200	-1.32879900
H	-3.71318100	1.55320900	-1.53985300
H	-3.59284800	-0.02193600	-2.32613800
C	-3.53026500	-1.93362100	-0.00006800
H	-3.13047400	-2.42492800	-0.88530600
H	-3.13049700	-2.42492500	0.88518300
H	-4.61700000	-2.01088600	-0.00008200
C	3.53025800	-1.93362700	-0.00002400
H	3.13036800	-2.42494700	-0.88521000
H	4.61699300	-2.01089600	-0.00015400
H	3.13058500	-2.42491500	0.88527900
C	3.94235300	0.49493100	1.43342500
H	5.01926200	0.36306200	1.32875200
H	3.71345000	1.55324400	1.53964500
H	3.59278100	-0.02180300	2.32608600
C	3.94227700	0.49499600	-1.43342800
H	3.71309600	1.55323700	-1.53976200
H	5.01921500	0.36341400	-1.32869000
H	3.59288400	-0.02191400	-2.32605800
Sn	-0.00000200	-1.63592300	-0.00003300

Compound XVIII′ (Singlet)

Absolute Energy = -2622.507301 a.u.

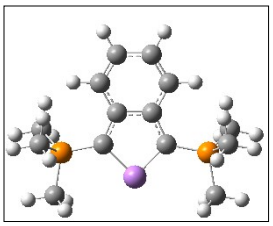


1 1

C	-0.54475000	1.28137900	-0.00028900
C	0.79766100	0.70740600	-0.00004600
C	0.79766400	-0.70740500	0.00006800
C	-0.54474300	-1.28138200	-0.00012200
C	1.97929800	-1.40102500	0.00034700
C	1.97929300	1.40102900	0.00011500
C	3.20461800	-0.68379700	0.00051300
C	3.20461500	0.68380400	0.00040800
H	4.13795000	-1.22870600	0.00072700
H	4.13794600	1.22871700	0.00054000
H	1.99403500	-2.48330100	0.00044300
H	1.99402800	2.48330500	0.00001300
As	-1.92721700	-0.00000200	-0.00023600
C	-0.76448000	2.73568000	-0.00010500
H	-0.27699200	3.18022200	0.87501200
H	-0.27461300	3.18127900	-0.87328200
H	-1.81541200	3.00793500	-0.00120900
C	-0.76447200	-2.73568200	0.00000000
H	-0.27560600	-3.18088100	-0.87397200
H	-0.27598000	-3.18062400	0.87432300
H	-1.81540400	-3.00793900	-0.00015800

Compound XVIII″ (Singlet)

Absolute Energy = -3464.834626 a.u.

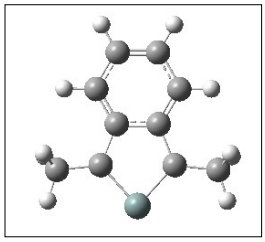


1 1

C	-1.28255700	-0.14063900	-0.00008900
C	-0.71352800	1.16931800	-0.00000600
C	0.71350200	1.16932500	0.00002700
C	1.28255000	-0.14062300	-0.00000200
C	1.39635300	2.40577400	0.00007500
C	-1.39638800	2.40576500	0.00001800
C	0.70320500	3.58824600	0.00010200
C	-0.70324500	3.58824100	0.00007500
H	1.23790900	4.52775700	0.00014400
H	-1.23795500	4.52774800	0.00008800
H	2.47869900	2.43488600	0.00009000
H	-2.47873500	2.43488100	-0.00002400
P	-2.98586700	-0.47713100	-0.00002600
P	2.98586100	-0.47712300	0.00005500
C	-3.82728200	0.17635500	1.45399900
H	-3.67369000	1.25083600	1.52710100
H	-4.89429400	-0.03602200	1.39480600
H	-3.40641600	-0.29752200	2.33953700
C	-3.82744800	0.17643400	-1.45392000
H	-4.89439200	-0.03629800	-1.39478100
H	-3.67420700	1.25098200	-1.52677900
H	-3.40642300	-0.29710800	-2.33956200
C	-3.26866100	-2.25199800	-0.00006400
H	-2.82448000	-2.69819800	-0.88828700
H	-2.82518400	-2.69812200	0.88854800
H	-4.34182800	-2.43899100	-0.00048500
C	3.26862100	-2.25199700	0.00000500
H	2.82464900	-2.69814600	-0.88834800
H	4.34178400	-2.43901000	-0.00015700
H	2.82491200	-2.69816000	0.88848300
C	3.82737100	0.17633300	1.45403900
H	4.89414800	-0.03739400	1.39543100
H	3.67510800	1.25105600	1.52634700
H	3.40554500	-0.29643300	2.33971100
C	3.82745800	0.17645800	-1.45381900
H	3.67454000	1.25106800	-1.52644100
H	4.89434700	-0.03660300	-1.39482700
H	3.40620300	-0.29678700	-2.33950900
As	0.00000400	-1.48765400	-0.00012600

Compound XIX′ (Singlet)

Absolute Energy = -676.283932 a.u.

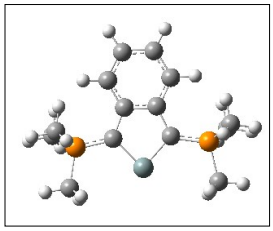


0 1

C	1.01385600	1.24546600	0.00009900
C	-0.36723000	0.70764200	0.00014500
C	-0.36722200	-0.70764300	0.00001300
C	1.01387400	-1.24545400	0.00006800
C	-1.54371400	-1.39789400	-0.00001500
C	-1.54372900	1.39788400	0.00028800
C	-2.77670900	-0.68130600	0.00028600
C	-2.77671700	0.68128600	0.00045900
H	-3.71005700	-1.22740700	0.00028300
H	-3.71007000	1.22737800	0.00065700
H	-1.55564500	-2.48058300	-0.00031200
H	-1.55566700	2.48057300	0.00029400
Si	2.38767800	0.00000500	0.00164700
C	1.17209000	-2.71896400	-0.00154700
H	0.67324900	-3.15574100	0.87191900
H	0.67324600	-3.15417000	-0.87577000
H	2.21579600	-3.02407900	-0.00177200
C	1.17207100	2.71897300	-0.00176700
H	0.67318100	3.15395500	-0.87607400
H	0.67327500	3.15597300	0.87161300
H	2.21577700	3.02408800	-0.00207100

Compound XIX″ (Singlet)

Absolute Energy = -1518.576841 a.u.



0 1

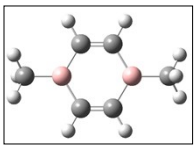
C	-1.27327800	0.35200300	0.00063100
C	-0.71465000	-0.98657000	0.00030700
C	0.71463000	-0.98657600	0.00010100
C	1.27327100	0.35199500	0.00014000
C	1.38701900	-2.21499600	-0.00001200
C	-1.38706000	-2.21497900	0.00027300
C	0.69569900	-3.41682800	-0.00005800

C	-0.69575500	-3.41681900	0.00006400
H	1.23906900	-4.35259800	-0.00015700
H	-1.23913600	-4.35258300	0.00004300
H	2.47121700	-2.24363100	-0.00001800
H	-2.47126000	-2.24360100	0.00047900
Si	0.00000500	1.68440700	0.00057100
P	-2.93971200	0.66131500	-0.00006900
P	2.93971400	0.66130200	-0.00006800
C	-3.85394700	0.01760600	-1.43330100
H	-3.68683800	-1.05416100	-1.52231800
H	-4.92192500	0.21476100	-1.34197000
H	-3.46370800	0.50078700	-2.32778200
C	-3.85536800	0.01746100	1.43220300
H	-4.92320100	0.21497600	1.33993300
H	-3.68870400	-1.05438000	1.52113100
H	-3.46582100	0.50031500	2.32716300
C	-3.28712200	2.43117900	-0.00004400
H	-2.84337000	2.88789600	0.88232800
H	-2.84394900	2.88787100	-0.88271500
H	-4.36525100	2.58854500	0.00030300
C	3.28707600	2.43117700	-0.00048200
H	2.84379500	2.88804900	0.88204400
H	4.36519700	2.58858800	-0.00075900
H	2.84338600	2.88768300	-0.88299300
C	3.85466900	0.01727700	-1.43270300
H	4.92241800	0.21568400	-1.34134200
H	3.68880000	-1.05474100	-1.52090300
H	3.46407100	0.49933500	-2.32763300
C	3.85476200	0.01778700	1.43273500
H	3.68834900	-1.05411300	1.52150700
H	4.92259600	0.21560200	1.34112900
H	3.46449700	0.50048400	2.32746400

.

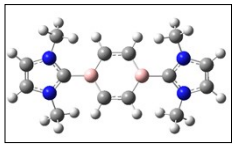
Compound XX′ (Singlet)

Absolute Energy = -284.203642 a.u.



0 1

C	-0.67120400	1.34715900	-0.00090000
C	0.67111700	1.34721000	0.00089200
C	0.67120400	-1.34715300	0.00089000
C	-0.67111600	-1.34720400	-0.00090300
H	-1.20238700	2.29807500	-0.00083400
1.20223100	2.29816300	0.00081700	
H	1.20238700	-2.29806900	0.00082000
H	-1.20223200	-2.29815700	-0.00083100
B	-1.47944100	-0.00005200	0.01831500
B	1.47944100	0.00005900	-0.01831700
C	3.04212500	0.00003100	-0.01212100
H	3.33873900	-0.00064600	1.04709600
H	3.49058100	-0.89129200	-0.45144000
H	3.49072400	0.89175900	-0.45045200
C	-3.04212500	-0.00003800	0.01213800
H	-3.33875100	0.00052000	-1.04707600
H	-3.49070200	-0.89173300	0.45055900
H	-3.49059400	0.89131800	0.45137700



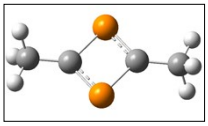
0 1

C	0.69528100	-1.11216700	0.67639400
C	-0.69535100	-1.11207300	0.67640400
C	-0.69526400	1.11174000	-0.67639900
C	0.69535400	1.11164500	-0.67644700
H	1.18730700	-1.91804900	1.22407000
H	-1.18751800	-1.91794800	1.22397500
H	-1.18735500	1.91765800	-1.22393800
H	1.18747400	1.91746200	-1.22415300
B	1.45876000	-0.00027900	0.00003000
B	-1.45877600	-0.00012800	0.00004200
C	-5.17684700	-0.67212600	-0.05191100
C	-5.17677700	0.67239700	0.05077600
C	-3.02751000	-0.00000500	-0.00007500
H	-5.98799000	-1.37457900	-0.10860400
H	-5.98787700	1.37490400	0.10741800
C	3.02740700	-0.00006800	0.00000400
C	5.17659500	0.67259400	0.05177300
C	5.17686800	-0.67188100	-0.05143500
H	5.98757400	1.37522900	0.10857800
H	5.98814200	-1.37415800	-0.10845600
N	3.85937800	1.07028700	0.08592000
N	3.85983000	-1.07007900	-0.08614000
N	-3.85965600	1.07025100	0.08552700
N	-3.85976800	-1.07021400	-0.08562200
C	3.43412000	-2.44660800	-0.24825500
H	3.34134400	-2.93968900	0.71796100
H	2.46317300	-2.45081100	-0.73730800
H	4.16993100	-2.96983800	-0.85580800
C	3.43313000	2.44667000	0.24795200
H	3.34033500	2.93975000	-0.71826400
H	2.46209700	2.45047700	0.73683400
H	4.16864000	2.97013000	0.85567200
C	-3.43343000	2.44668200	0.24715600

H	-2.46319300	2.45079800	0.73761900
H	-3.33883000	2.93893300	-0.71929200
H	-4.16993600	2.97078800	0.85309600
C	-3.43350500	-2.44677800	-0.24601500
H	-2.46311900	-2.45124200	-0.73619000
H	-3.33921100	-2.93827200	0.72086700
H	-4.16981700	-2.97136300	-0.85177100

Compound XXI′ (Singlet)

Absolute Energy = -838.561406 a.u.

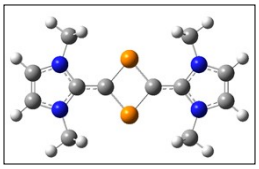


0 1

C	1.17227100	0.02253200	0.00055900
C	-1.17237900	-0.02224500	-0.00037900
P	-0.15707400	-1.34152000	-0.00002600
P	0.15718900	1.34139700	-0.00001700
C	2.64470700	-0.11988900	0.00000000
H	3.14867400	0.84712900	-0.00002500
H	2.97614600	-0.68691500	0.87479600
H	2.97495900	-0.68553500	-0.87639900
C	-2.64482300	0.11992700	-0.00002700
H	-2.97624800	0.68682200	-0.87491500
H	-3.14858600	-0.84719600	-0.00000400
H	-2.97533100	0.68558300	0.87627400

Compound XXI″ (Singlet)

Absolute Energy = -1368.275178 a.u.



0 1

C	4.70528800	0.67287600	-0.00003200
C	4.70528500	-0.67288500	0.00029800
C	2.55575300	-0.00000400	-0.00005800
H	5.51748700	1.37588400	-0.00015600
H	5.51748500	-1.37589100	0.00054900
C	-2.55576400	0.00000600	0.00003500
C	-4.70528500	-0.67289900	-0.00018900
C	-4.70530500	0.67285900	0.00009800
H	-5.51746600	-1.37592700	-0.00035300
H	-5.51749900	1.37587100	0.00018300
N	-3.38873100	-1.08424900	-0.00020600
N	-3.38875600	1.08423900	0.00024600
N	3.38874100	-1.08424600	0.00028400
N	3.38874200	1.08423800	-0.00031400
C	-2.93993100	2.45735100	0.00060200
H	-2.33000600	2.65257700	0.88267300
H	-2.33086700	2.65336200	-0.88188700
H	-3.81352000	3.10393700	0.00130500
C	-2.93988100	-2.45735500	-0.00055400
H	-2.33009400	-2.65264300	-0.88270300
H	-2.33068000	-2.65328000	0.88185900
H	-3.81346400	-3.10395000	-0.00107000
C	2.93993000	-2.45737200	0.00047800
H	2.33073100	-2.65298200	0.88295300
H	2.33016800	-2.65302300	-0.88161500
H	3.81353900	-3.10392800	0.00017200
C	2.93992800	2.45736300	-0.00071000
H	2.32961800	2.65238600	-0.88255200
H	2.33125500	2.65358300	0.88200700
H	3.81353100	3.10392400	-0.00192800
C	-1.16203300	0.00001900	0.00011000
C	1.16202100	0.00000700	-0.00013800
P	0.00001200	1.35347900	0.00007600
P	-0.00002700	-1.35345100	-0.00002000

Compound XXII′ (Singlet)

Absolute Energy = -727.965932 a.u.

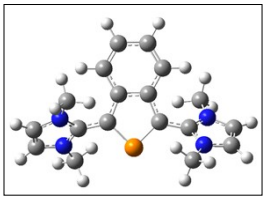
1 1

C	-0.97134300	1.23362500	0.00035000
C	0.39203300	0.70553600	0.00026200
C	0.39311700	-0.70516200	0.00020300
C	-0.96858300	-1.23511000	0.00030800
C	-1.24579200	-2.68001000	0.00005600
C	-1.24960200	2.67847200	0.00003000
P	-2.22164200	-0.00110300	-0.00005400
C	1.56969800	-1.40469500	0.00004900
C	1.56739500	1.40653300	0.00001100
C	2.79294700	-0.68251400	-0.00011300
C	2.79179600	0.68582000	-0.00011700

H	3.72779400	-1.22478000	-0.00051400
H	3.72585600	1.22948000	0.00002200
H	1.58415200	-2.48705200	0.00053000
H	1.58050700	2.48889800	-0.00030700
H	-0.78300300	3.13965900	-0.87763600
H	-2.31133100	2.90560600	0.00486400
H	-0.77345300	3.14293300	0.87060600
H	-0.77172300	-3.14438900	0.87168500
H	-2.30740700	-2.90795100	0.00190000
H	-0.77675100	-3.14082700	-0.87657200

Compound XXII″ (Singlet)

Absolute Energy = -1257.770409 a.u.

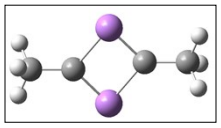


1 1

C	-1.23631100	0.20692200	0.07840900
C	-0.70857400	-1.12029900	0.05040100
C	0.70857400	-1.12030600	-0.05046900
C	1.23630700	0.20692800	-0.07838000
C	2.64481400	0.49928000	-0.07740100
C	4.80006000	0.53792000	0.48201600
C	4.63801500	1.35387500	-0.58071700
H	5.67732200	0.28560500	1.04910900
H	5.34708400	1.94884100	-1.12640000
N	3.30494000	1.31620300	-0.92063600
N	3.56199300	0.02149100	0.78860700
C	2.71732200	2.03366100	-2.04413900
H	1.89368800	1.44737300	-2.44129600
H	2.34673500	3.00471000	-1.72391300
H	3.48252100	2.16309200	-2.80424600
C	3.28019600	-0.80909100	1.95194900
H	3.51597400	-1.85057700	1.74670300
H	3.88056300	-0.45061300	2.78372200
H	2.22442900	-0.72249700	2.19092100
C	-2.64481600	0.49926000	0.07741200
C	-4.63804600	1.35379300	0.58071300
C	-4.80002600	0.53797800	-0.48213800
H	-5.34714700	1.94870000	1.12642100
H	-5.67725000	0.28574900	-1.04932800
N	-3.56194700	0.02156100	-0.78869800
N	-3.30498900	1.31608400	0.92070300
C	-3.28006100	-0.80891600	-1.95209100
H	-2.22433600	-0.72205300	-2.19116400
H	-3.51555700	-1.85047000	-1.74687100
H	-3.88059600	-0.45055000	-2.78379000
C	-2.71744000	2.03337900	2.04434500
H	-2.34687000	3.00449100	1.72429000
H	-3.48266800	2.16266300	2.80444600
H	-1.89380100	1.44705500	2.44143900
P	0.00000100	1.42373000	0.00010500
C	1.39591100	-2.34707500	-0.14502100
C	-1.39592600	-2.34707600	0.14495200
C	0.69946300	-3.52829400	-0.08269700
C	-0.69947600	-3.52829500	0.08262700
H	1.22577200	-4.46971900	-0.15872000
H	-1.22576800	-4.46972700	0.15869700
H	2.46996000	-2.35864800	-0.28789100
H	-2.46997400	-2.35862200	0.28782500

Compound XXIII′ (Singlet)

Absolute Energy = -4627.645192 a.u.

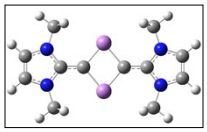


0 1

C	1.16941400	0.39673100	0.00003100
C	-1.16895200	-0.39686700	-0.00003900
C	2.50795900	1.02586900	-0.00046000
H	2.62613100	1.67279400	-0.87559100
H	2.62664800	1.67329000	0.87423200
H	3.31448400	0.29128100	-0.00051400
C	-2.50752100	-1.02607400	-0.00045400
H	-2.62571000	-1.67309000	-0.87550200
H	-2.62616100	-1.67340200	0.87432000
H	-3.31406600	-0.29151400	-0.00051700
As	0.64422100	-1.31562200	0.00013800
As	-0.64442500	1.31570300	0.00013800

Compound XXIII″ (Singlet)

Absolute Energy = -5157.365195 a.u.



0 1

C	4.78187600	0.67263200	0.00001900

C	4.78189500	-0.67255500	0.00048000
C	2.62647800	0.00001200	-0.00004300
H	5.59463700	1.37504300	-0.00011300
H	5.59466300	-1.37495600	0.00087000
C	-2.62648800	-0.00000800	-0.00004200
C	-4.78188300	-0.67264800	-0.00010700
C	-4.78190700	0.67254400	0.00036500
H	-5.59465100	-1.37505100	-0.00041600
H	-5.59470200	1.37491500	0.00059400
N	-3.46585200	-1.08481900	-0.00036500
N	-3.46589100	1.08477200	0.00031700
N	3.46586600	-1.08477100	0.00048600
N	3.46584700	1.08481900	-0.00029500
C	-3.02583600	2.45897600	0.00108200
H	-2.41955300	2.66071700	0.88481400
H	-2.42035600	2.66203900	-0.88289400
H	-3.90303000	3.10063100	0.00195400
C	-3.02567700	-2.45898200	-0.00062000
H	-2.41955300	-2.66106700	-0.88438000
H	-2.41996300	-2.66156200	0.88331800
H	-3.90280500	-3.10072400	-0.00101900
C	3.02578300	-2.45895700	0.00086200
H	2.41949200	-2.66096600	0.88453100
H	2.42029300	-2.66173600	-0.88317400
H	3.90295300	-3.10064700	0.00157500
C	3.02571000	2.45898700	-0.00083200
H	2.41937300	2.66082300	-0.88451000
H	2.42024600	2.66188000	0.88319500
H	3.90285300	3.10071400	-0.00168600
C	-1.23579600	-0.00002400	0.00003400
C	1.23578500	0.00001500	-0.00029400
As	-0.00002900	1.46088500	-0.00013100
As	0.00004900	-1.46088500	-0.00014400

Coordinates of 4g

37
symmetry c2v
E = -967.920579539

C	-1.061815000	0.000000000	1.153402000
C	-0.689213000	0.000000000	2.517055000
C	0.689213000	0.000000000	2.517055000
C	1.061815000	0.000000000	1.153402000
N	0.000000000	0.000000000	0.326885000
H	-1.334943000	0.000000000	3.380411000
H	1.334943000	0.000000000	3.380411000
C	-2.370095000	0.000000000	0.589541000
C	-4.592022000	0.000000000	0.319555000
C	-3.998773000	0.000000000	-0.943790000
N	-2.626968000	0.000000000	-0.722746000
N	-3.544389000	0.000000000	1.236581000
C	2.370095000	0.000000000	0.589541000
C	3.998773000	0.000000000	-0.943790000
C	4.592022000	0.000000000	0.319555000
N	3.544389000	0.000000000	1.236581000
N	2.626968000	0.000000000	-0.722746000
C	5.968190000	0.000000000	0.480557000
C	4.758070000	0.000000000	-2.103276000
C	6.132882000	0.000000000	-1.944331000
C	6.726668000	0.000000000	-0.677057000
H	6.427383000	0.000000000	1.458705000
H	7.804414000	0.000000000	-0.600338000
H	6.764239000	0.000000000	-2.821191000
H	4.301063000	0.000000000	-3.082311000
C	-4.758070000	0.000000000	-2.103276000
C	-5.968190000	0.000000000	0.480557000
C	-6.726668000	0.000000000	-0.677057000
C	-6.132882000	0.000000000	-1.944331000
H	-4.301063000	0.000000000	-3.082311000
H	-6.764239000	0.000000000	-2.821191000
H	-7.804414000	0.000000000	-0.600338000
H	-6.427383000	0.000000000	1.458705000
H	3.630920000	0.000000000	2.239539000
H	1.881193000	0.000000000	-1.401770000
H	-1.881193000	0.000000000	-1.401770000
H	-3.630920000	0.000000000	2.239539000

References:

1. G. K. Pierens, *J. Comput. Chem.* , 2014, **35**, 1388-1394.
2. M. Begtrup, *J. Chem. Soc., Chem. Commun.*, 1975, DOI: 10.1039/C39750000334, 334-335.
3. M. C. Cann, *J. Org. Chem.*, 1988, **53**, 1112-1113.
4. G. Boche, P. Andrews, K. Harms, M. Marsch, K. S. Rangappa, M. Schimeczek and C. Willeke, *J. Am. Chem. Soc.*, 1996, **118**, 4925-4930.
5. T. Soos, G. Hajós and A. Messmer, *J. Org. Chem.*, 1997, **62**, 1136-1138.
6. S. McIlroy, C. J. Cramer and D. E. Falvey, *Org. Lett.*, 2000, **2**, 2451-2454.
7. K. Satake, Y. Kubota, C. E. Cordonier, H. Okamoto and M. Kimura, *Angew. Chem. Int. Ed.*, 2004, **43**, 736-738.
8. A. H. Winter, H. H. Gibson and D. E. Falvey, *J. Org. Chem.*, 2007, **72**, 8186-8195.
9. J. L. Crandon and D. P. Nicolau, *Antimicrob. Agents Chemother.*, 2015, **59**, 2688-2694.
10. A. Pogoreltsev, Y. Tulchinsky, N. Fridman and M. Gandelman, *J. Am. Chem. Soc.*, 2017, **139**, 4062-4067.
11. J. Zhou, L. L. Liu, L. L. Cao and D. W. Stephan, *Chem. Commun.*, 2018, **54**, 4390-4393.
12. J. Zhou, L. L. Liu, L. L. Cao and D. W. Stephan, *Angew. Chem. Int. Ed.* , 2018, **57**, 3322-3326.
13. G. M. Peters, J. B. Winegrad, M. R. Gau, G. H. Imler, B. Xu, S. Ren, B. B. Wayland and M. J. Zdilla, *Inorg. Chem.*, 2017, **56**, 3377-3385.
14. D. Xue and Y.-Q. Long, *J. Org. Chem.*, 2014, **79**, 4727-4734.
15. M. L. P. R. Alapati, S. R. Abburi, S. B. Mukkamala and R. M. Krishnaji, *Syn. Commun.*, 2015, **45**, 2436-2443.
16. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
17. M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi and R. Spagna, *J. Appl. Crystallogr.*, 2007, **40**, 609-613.
18. G. M. Sheldrick, *Acta Crystallogr. C*, 2015, **71**, 3-8.

19. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Journal*, 2016, Gaussian, Inc.: Wallingford, CT.
20. T. Ziegler and A. Rauk, *Inorg. Chem.*, 1979, **18**, 1755-1759.
21. K. Morokuma, *J. Chem. Phys.*, 1971, **55**, 1236-1244.
22. M. Mousavi and G. Frenking, *Organometallics*, 2013, **32**, 1743-1751.
23. M. v. Hopffgarten and G. Frenking, *WIREs Comput. Mol. Sci.*, 2012, **2**, 43-62.
24. T. A. N. Nguyen and G. Frenking, *Chem. Eur. J.*, 2012, **18**, 12733-12748.
25. K. Kitaura and K. Morokuma, *Int. J. Quantum Chem.* , 1976, **10**, 325-340.
26. T. Ziegler and A. Rauk, *Theor. Chim. Acta* 1977, **46**, 1-10.
27. M. P. Mitoraj, A. Michalak and T. Ziegler, *J. Chem. Theory Comput.*, 2009, **5**, 962-975.
28. M. Mitoraj and A. Michalak, *J. Mol. Model.*, 2008, **14**, 681-687.
29. A. Michalak, M. Mitoraj and T. Ziegler, *J. Phys. Chem. A*, 2008, **112**, 1933-1939.
30. M. Mitoraj and A. Michalak, *Organometallics*, 2007, **26**, 6576-6580.
31. M. Mitoraj and A. Michalak, *J. Mol. Model.*, 2007, **13**, 347-355.
32. ADF2020.102, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, see http://www.scm.com, (accessed October 5, 2024).
33. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931-967.