Supporting Information

Donor-Acceptor Assisted Alkyne Hydration: A Luminescent Boron-Stabilized Enol

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Content

S1. Materials and Methods

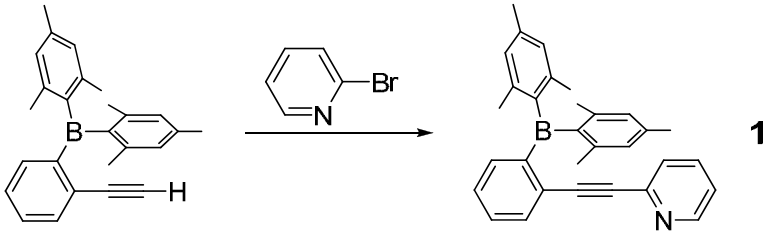
General Procedure. All experiments were performed under a nitrogen atmosphere in a Vacuum Atmospheres drybox or by standard Schlenk technique unless otherwise noted. THF was dried and distilled over sodium benzophenone ketyl prior to use. Methylene chloride was dried and distilled over P_2O_5 as solvent for photophysical measurements. Thin-layer and flash chromatography were performed on silica gel. ^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance spectrometers, and deuterated solvents were purchased from Cambridge Isotopes and used without further drying. High resolution mass spectra (HRMS) were obtained from an Applied Biosystems QStar XL spectrometer. 1-Dimesitylboryl-2-ethynylbenzene was synthesized according to a literature procedure.[2]

Electrochemical and Photophysical Measurements. Cyclic voltammetry experiments were performed using a BAS CV-50W analyzer with a scan rate of 0.1-0.2 V/sec using 2 mg sample in 0.5 mL dry DMF. The electrochemical cell was a standard three-compartment cell composed of a Pt working electrode, a Pt auxiliary electrode, and an Ag/AgCl reference electrode. CV measurements were carried out at room temperature with 0.1 M tetrabutylammonium hexafluorophosphate (TBAP) as the supporting electrolyte. Excitation and emission spectra were recorded using a Photon Technologies International QuantaMaster Model 2 spectrometer (CH_2Cl_2 at 1×10^{-5} M). UV/Visible spectra were recorded using a Varian Cary 50Bio UV-vis spectrophotometer. Photoluminescent quantum yields were measured using optically dilute method (1×10^{-5} M, A $\approx$ 0.1) at room temperature in CH_2Cl_2 relative to anthracene (Φr = 0.36). The fluorescence quantum yields were calculated using previously known procedures.[1]

Density Functional Theory Calculations. Molecular orbital and molecular geometry calculations were performed using the Gaussian 03 program suite using crystal structures as the starting point for geometry optimizations where possible. Calculations were performed at the B3LYP level of theory using 6-31G* as the basis set.

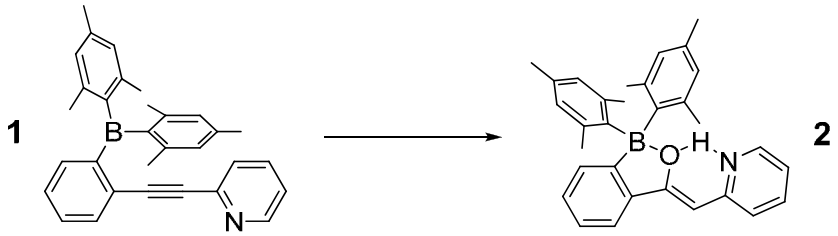
S2. **Synthetic Procedures and Characterization**

Preparation of 2-(2'-(dimesitylboryl)phenylethynyl)pyridine (1)



1-Dimesitylboryl-2-ethynylbenzene (0.326 g, 0.93 mmol), 2-bromopyridine (0.176 g, 1.12 mmol), $Pd(PPh_3)_2Cl_2$ (0.039 g, 0.056 mmol) and CuI (0.009 g, 0.046 mmol) in THF (15 mL) and Et_3N (0.2 mL) were reacted overnight at 70°C under N_2. THF was evaporated *in vacuo* and the residue was extracted using CH_2Cl_2/5% aq. NH_4Cl. The organic layer was dried over $MgSO_4$, concentrated, and the residue purified by column chromatography on silica (15:1 hexanes:EtOAc) to afford **1** as a white solid (0.141 g, 35%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50 (d, J = 4.3 Hz, 1H, pyridine), 7.66 (d, J = 7.6 Hz, 1H, phenyl), 7.48 (dt, J = 7.8 Hz, J = 1.5 Hz, 1H, pyridine), 7.40 (dt, J = 7.6 Hz, J = 1.8 Hz, 1H, pyridine), 7.30 (m, 2H, phenyl), 7.10 (dt, J = 6.7 Hz, J = 1.6 Hz, 1H, phenyl), 6.76 (s, 4H, mesityl), 6.68 (d, J = 7.8 Hz, 1H, pyridine), 2.24 (s, 6H, mesityl), 2.02 (s, 12H, mesityl). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.1, 143.3, 142.8, 140.9, 139.0, 135.7, 134.5, 133.5, 130.4, 128.6, 128.3, 127.4, 126.0, 122.2, 91.0, 90.5, 23.2, 21.2 ppm. HRMS calc'd for $C_{31}H_{30}BN$ [M^+] 427.2471, found 427.2482.

Preparation of Compound 2

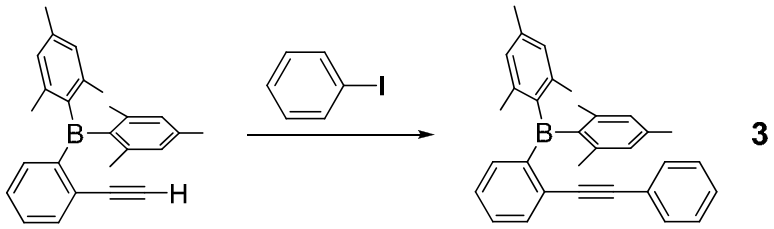


Isolation of compound 2 from the initial Sonogashira coupling reaction: 1-dimesitylboryl-2-ethynylbenzene (0.630 g, 1.80 mmol), 2-bromopyridine (0.341 g, 2.16 mmol), $Pd(PPh_3)_2Cl_2$ (0.076 g, 0.108 mmol) and CuI (0.017 g, 0.090 mmol) in THF/Et_3N (5:1) were reacted overnight at 70°C under N_2. THF was evaporated *in vacuo* and the residue was extracted using CH_2Cl_2/5% aq. NH_4Cl. The resulting precipitate was separated from the liquid organic layer and purified by column chromatography on silica (1:1 hexanes:CH_2Cl_2) to afford **2** as a yellow solid (0.180 g, 22%). ^{1}H NMR (C_6D_6, 400 MHz): δ 14.1 (s, br, pyridinium), 8.13 (d, J = 7.5 Hz, 1H, pyridine), 7.58 (d, J = 7.7 Hz, 1H, pyridine), 7.24 (t, J = 7.5 Hz, 1H, pyridine), 7.14, (t, J = 7.7 Hz, 1H, pyridine), 6.92 (s, 4H, mesityl), 6.32 (t, J = 8.6 Hz, 1H, phenyl), 6.14 (t, J = 6.0, 1H, phenyl), 5.96 (d, J = 8.9 Hz, 1H, phenyl), 5.57 (s, 1H, vinyl), 5.42 (t, J = 6.7 Hz, 1H, phenyl), 2.42 (s, 12H,

mesityl), 2.29 (s, 6H, mesityl) ppm; ^{13}C NMR (CD_2Cl_2, 75 MHz): δ 179.8, 155.3, 141.8, 140.6, 137.9, 135.4, 133.8, 132.2, 131.2, 129.6, 125.6, 124.7, 124.1, 122.2, 116.4, 85.0, 24.9, 21.0 ppm. HRMS calc'd for $C_{31}H_{32}BNO$ [M^+] 445.2577, found 445.2570.

NMR scale reaction showing the conversion of 1 to 2 using CuI as the catalyst: CD_2Cl_2 (5 mL) was added to a vial containing **1** (0.010 g, 0.023 mmol) and CuI (0.447 mg, 0.002 mmol) inside a glovebox. The sealed vial was then removed from the glovebox to allow the addition of 10 eq. H_2O (4.0 μL, 0.233 mmol) under N_2. The mixture was stirred under inert atmosphere at room temperature and monitored by ^{1}H NMR. The conversion yield was determined by NMR, integrating the aromatic dimesityl proton peak of **2** in reference to that of **1** (see **Figure S12a**). After 3 days, ^{1}H NMR spectra showed 40% conversion of **1** to **2**.

Preparation of 2-(2'-(dimesitylboryl)phenylethynyl)benzene (3)



3

Prepared in analogy to **1**: 1-dimesitylboryl-2-ethynylbenzene (0.080 g, 0.23 mmol), iodobenzene (0.056 g, 0.27 mmol), $Pd(PPh_3)_2Cl_2$ (0.010 g, 0.014 mmol) and CuI (0.002 g, 0.011 mmol) in THF (10 mL) and Et_3N (0.16 mL) was reacted overnight at 50^{o}C under N_2. The crude product was purified by column chromatography on silica (50:1 hexanes:EtOAc) to afford **3** as a white solid. The purity of **3** was further improved by crystallization in CH_2Cl_2 and hexanes, yield 45%. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ 7.55 (d, J = 7.6 Hz, 1H, borylphenyl), 7.41, (dt, J = 7.4 Hz, J = 1.6 Hz, 1H, borylphenyl), 7.29 (dt, J = 7.3 Hz, J = 1.2 Hz, 1H, borylphenyl), 7.25, (d, J = 7.6 Hz, 2H, phenyl), 7.22 (m, 2H, phenyl), 7.02 (dd, J = 7.6 Hz, J = 1.9 Hz, 2H, phenyl), 6.78 (s, 4H, mesityl), 2.26 (s, 6H, mesityl), 2.00 (s, 12H, mesityl) ppm. ^{13}C NMR (CD_2Cl_2, 100 MHz): 143.4, 141.3, 139.7, 134.9, 133.4, 132.0, 130.8, 128.8, 128.3 128.4, 127.6, 123.9, 92.8, 90.6, 23.4, 21.5 ppm. HRMS calc'd for $C_{32}H_{31}B$ [M^+] 426.2519, found 426.2531.

S3. ^{1}H NMR Spectra

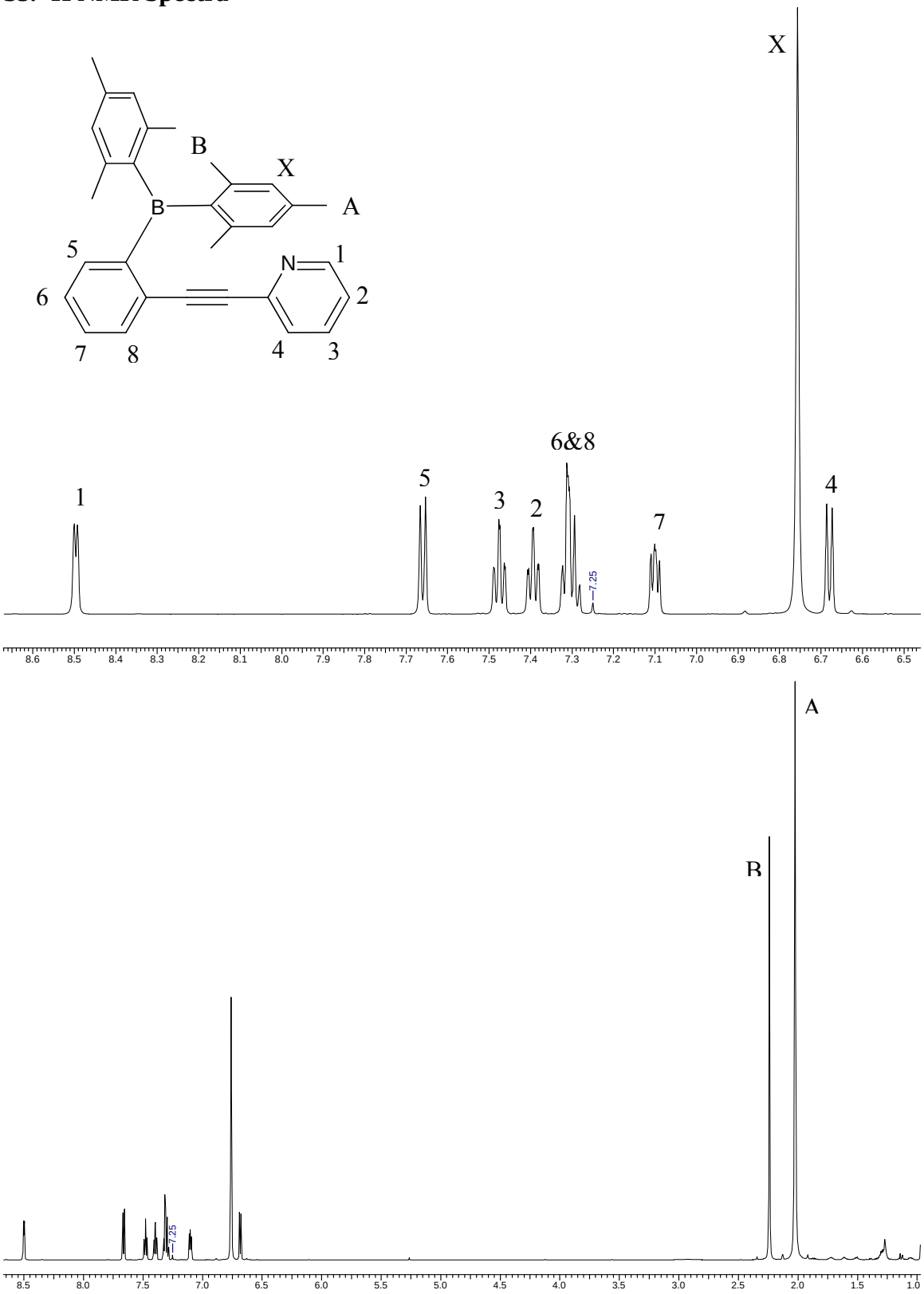


Figure S1. The full spectrum of **1** in $CDCl_3$ (bottom) and the expanded aromatic region (top).

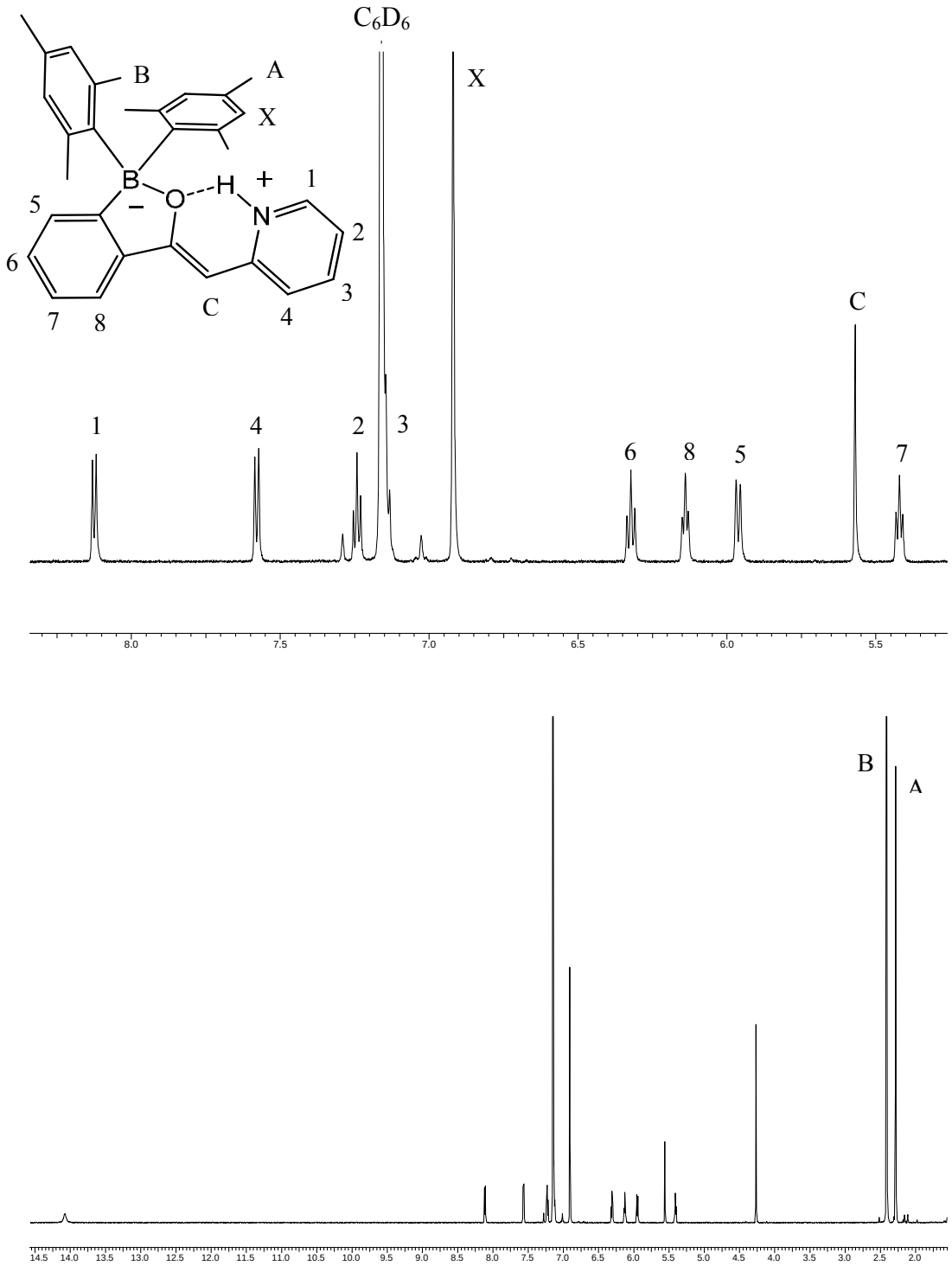


Figure S2. The full ^{1}H NMR spectrum of **2** in C_6D_6 (bottom) and the expanded aromatic region (top).

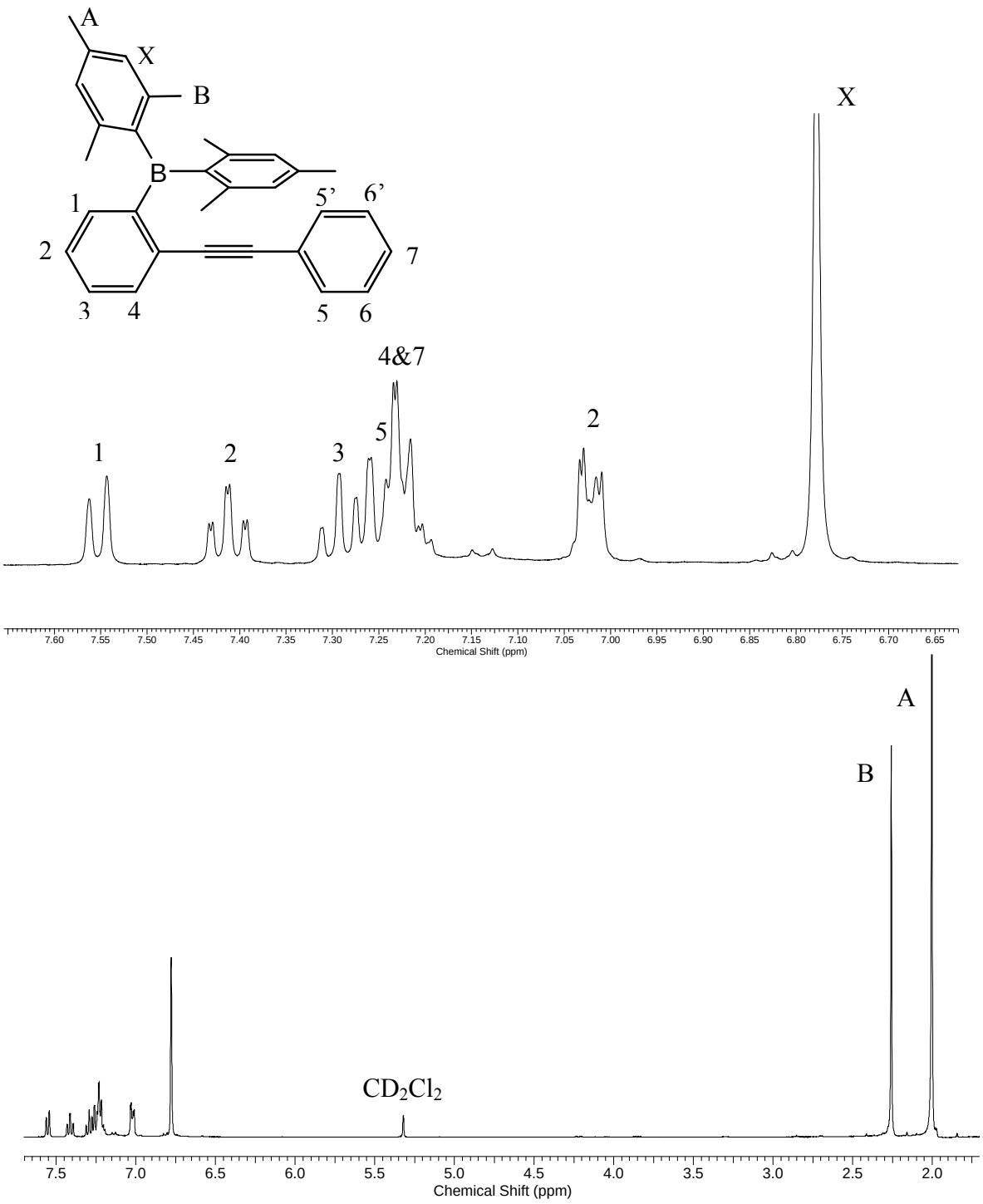


Figure S3. The full ^{1}H spectrum of **3** in CD_2Cl_2 (bottom) and the expanded aromatic region (top).

S4. Absorption and Emission Spectra

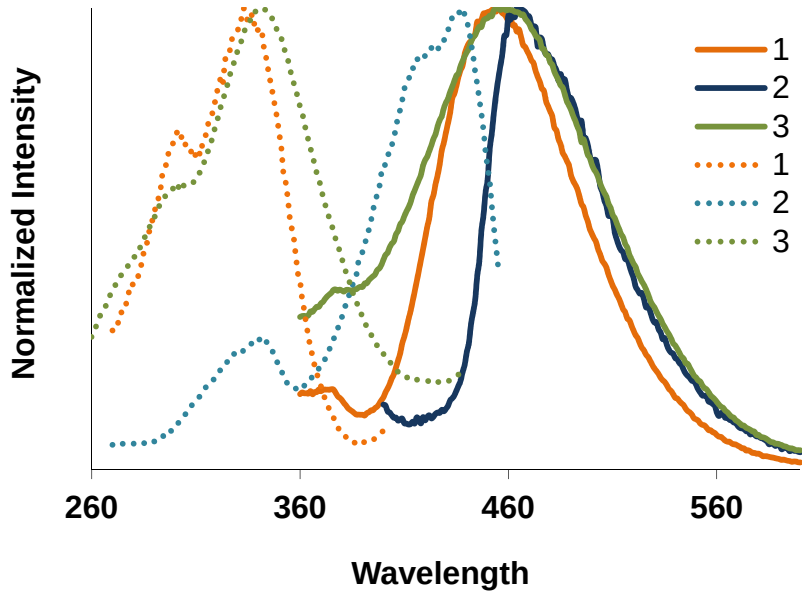


Figure S4. Emission (solid lines) and (dotted lines) excitation spectra (in CH_2Cl_2).

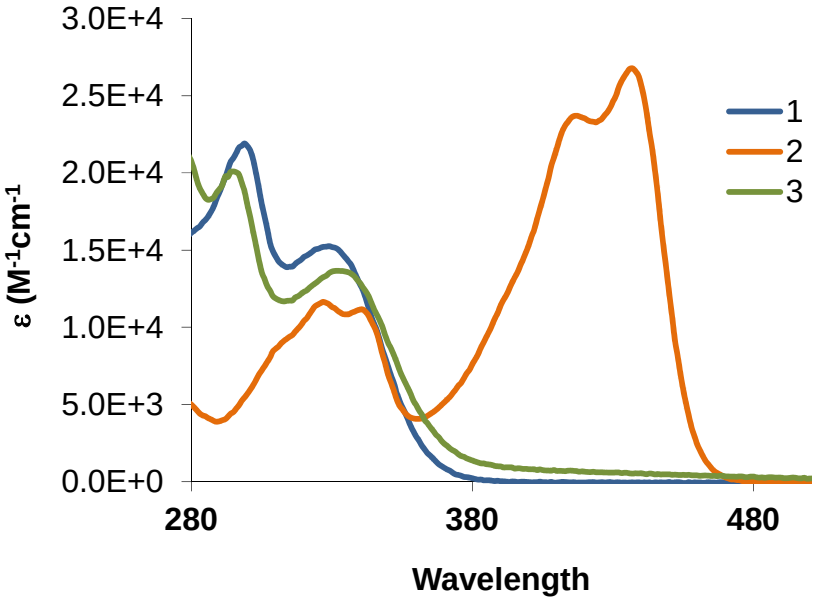


Figure S5. Absorption spectra of the three compounds in 10^{-5} M solutions in CH_2Cl_2.

Table 1. Photophysical and Electrochemical Properties of **1-3**

Complex	Absorption, λ_{max} ε (10^4 cm^{-1} M^{-1})	Solution Emission, 298K λ_{max} (nm)	Φ_P	$E_{1/2}^{red}$ (V) (vs. $FeCp_2^{+/0}$)
1	297 (2.2), 326 (1.5)	455	0.04	-2.22
2	331 (1.1), 435 (2.7)	464	0.04	--
3	298 (1.9), 340 (1.3)	455	0.04	-2.29

S5. Cyclic Voltammetry Diagrams

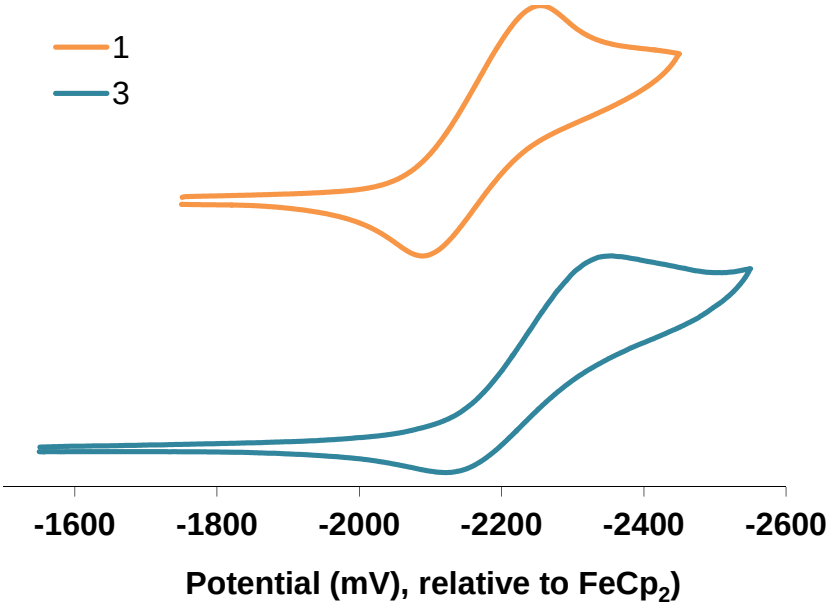


Figure S6. Cyclic voltammetry diagrams of **1** and **3** in DMF.

S6. Response of **1** and **3** to fluoride

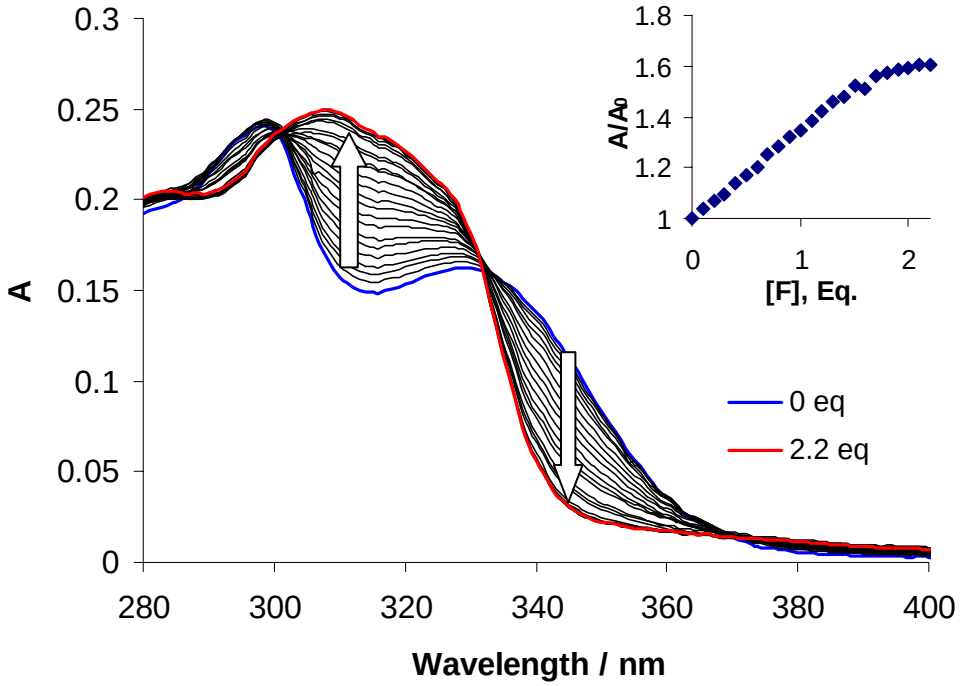


Figure S7a. The UV-Vis titration of **1** by NBu_4F in CH_2Cl_2 (1.0×10^{-5} M). Inset: the Stern-Volmer plot at 312 nm.

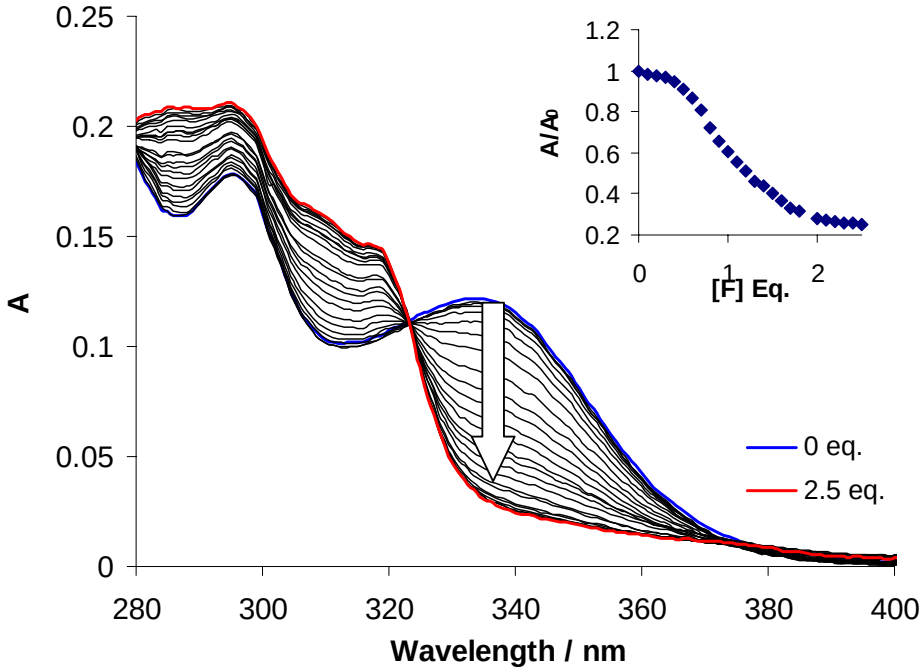
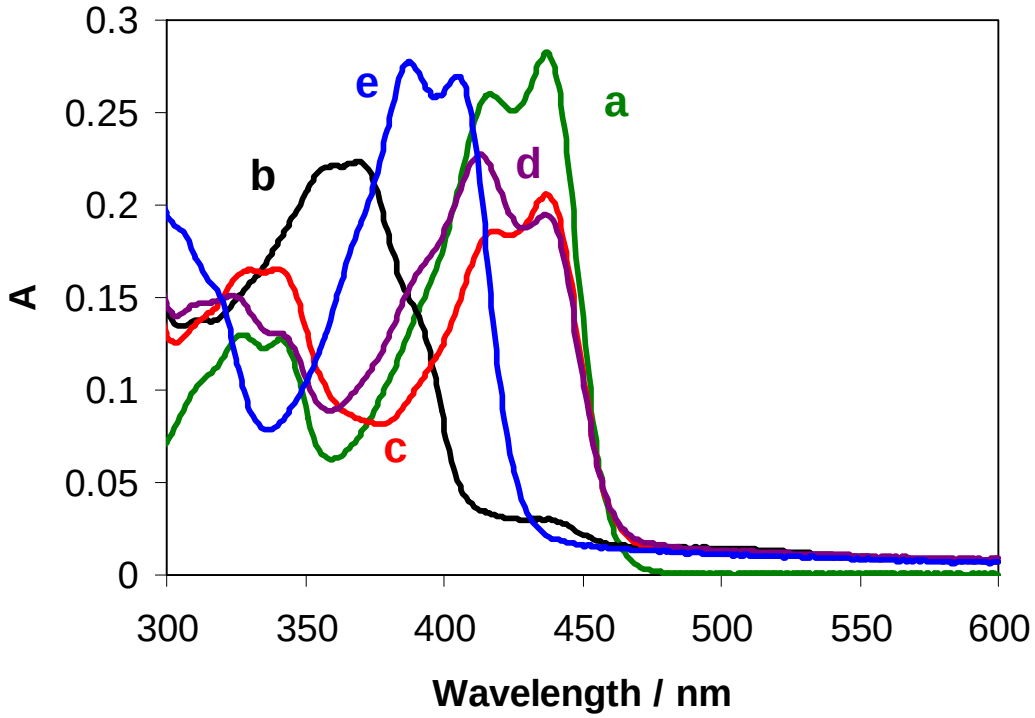


Figure S7b. The UV-Vis titration of **3** by NBu_4F in CH_2Cl_2 (1.0×10^{-5} M). Inset: The Stern-Volmer plot at 335 nm.

S7. The UV-Vis spectral change of compound **2** with the addition of NaOMe and the subsequent addition of HBF_4 in CH_2Cl_2. (a) compound **2**, (b) compound **2** + 24 eq. NaOMe, (c) the solution of (b) + 2 eq. HBF_4 (d) the solution of (b) + 24 eq. HBF_4, (d) the solution of (b) + 60 eq. HBF_4.



S8. Density Functional Theory Calculations

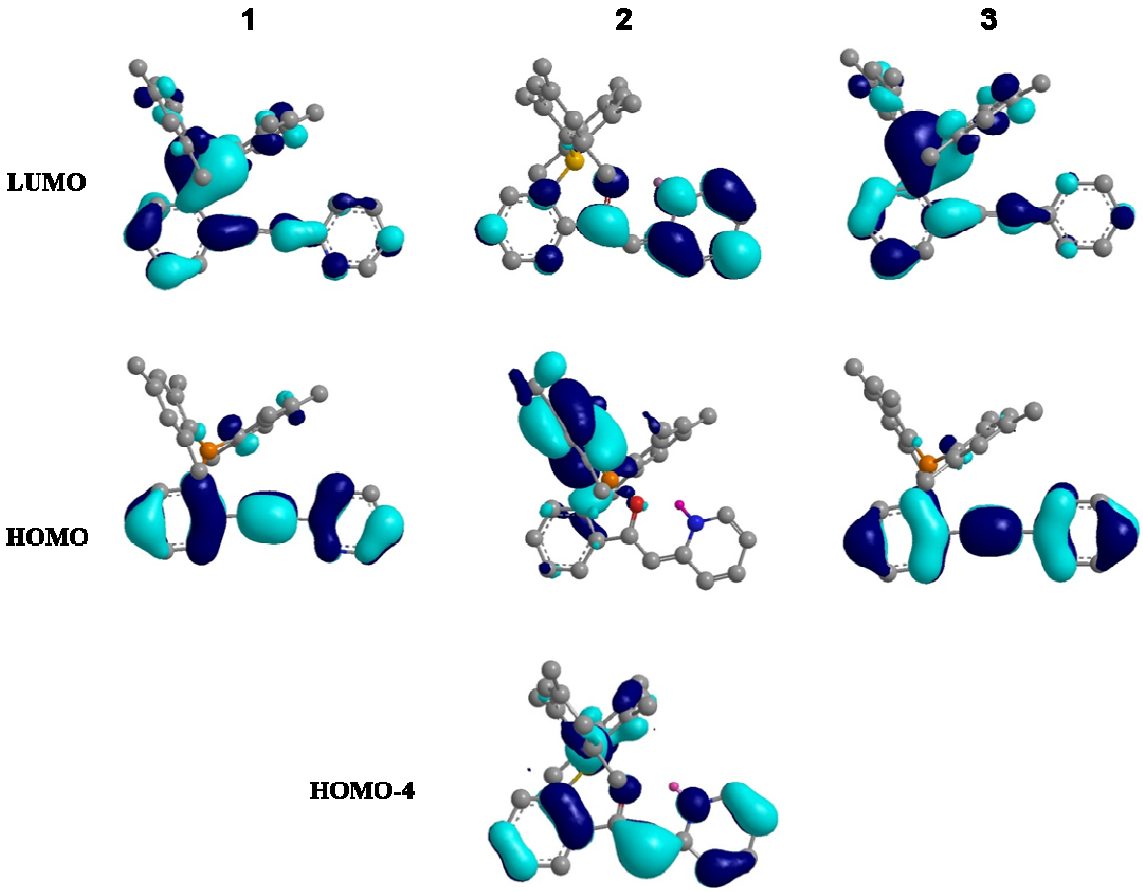


Figure S8. HOMO and LUMO molecular orbitals of **1**, **2** and **3**.

Table 2. TD-DFT Results

Compound 1

Excited State	Transition	Energy (eV)	*f*	Optical Energy Gap from UV-vis spectra (eV)
1	HOMO → LUMO HOMO-1 → LUMO	3.32	0.0874	3.31
2	HOMO-1 → LUMO HOMO→ LUMO	3.43	0.1453	
3	HOMO-2 → LUMO HOMO-3 → LUMO	3.68	0.0121	
4	HOMO-3 → LUMO HOMO-2 → LUMO	3.72	0.0295	
5	HOMO-4 → LUMO	3.73	0.0122	
6	HOMO → LUMO+1 HOMO-1 → LUMO+1	4.11	0.3345	

Compound 2

1	HOMO → LUMO	2.52	0.0089	2.66
2	HOMO-1 → LUMO	2.67	0.0076	
3	HOMO-2 → LUMO	2.85	0.0032	
4	HOMO-3 → LUMO	2.93	0.0033	
5	HOMO-4 → LUMO ($\pi \rightarrow \pi^*$)	3.11	0.2331	
6	HOMO → LUMO+1	3.26	0.0177	
7	HOMO-1 → LUMO+1	3.39	0.0265	
8	HOMO-2 → LUMO+1 HOMO-3 → LUMO+1	3.57	0.0205	
9	HOMO-5 → LUMO HOMO-4 → LUMO+1 HOMO-3 → LUMO+1	3.61	0.0481	
10	HOMO-3 → LUMO+1 HOMO-5 → LUMO HOMO-4 → LUMO+1	3.65	0.008	
11	HOMO-4 → LUMO+1 HOMO-5 → LUMO	3.75	0.3879	

Compound 3

1	HOMO → LUMO	3.24	0.1158	3.27
2	HOMO-1 → LUMO	3.43	0.1078	
3	HOMO-2 → LUMO HOMO-3 → LUMO	3.69	0.0110	
4	HOMO-3 → LUMO HOMO-4 → LUMO	3.74	0.0325	
5	HOMO-4 → LUMO	3.75	0.0142	

	HOMO-3 → LUMO			
6	HOMO → LUMO+1 HOMO-5 → LUMO	4.15	0.3887	
7	HOMO-1 → LUMO+1 HOMO-7 → LUMO HOMO-5 → LUMO	4.25	0.0421	
8	HOMO-5 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+1	4.42	0.1905	

S9. TD-DFT Calculated and experimental absorption spectra for [2]$^-$

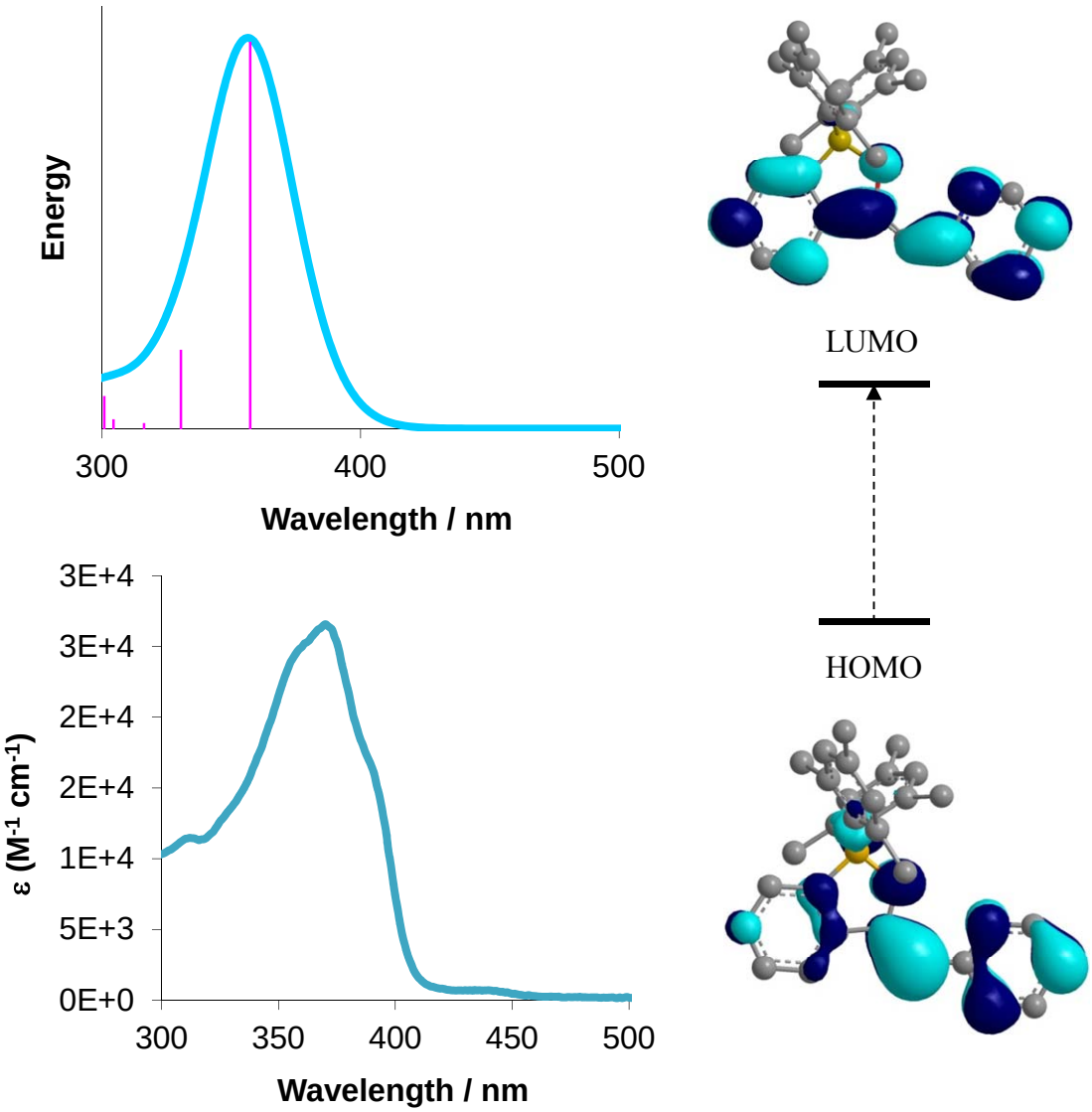


Figure S9. Left: energy spectrum calculated using time-dependent DFT for [**2**]$^-$ (top) and absorbance spectrum of **2** at the endpoint of NaOMe titration (bottom). Right: the corresponding MOs responsible for the lowest energy transition band in the UV-Vis spectrum (HOMO-LUMO gap calculated from TD-DFT is 3.42 eV).

S10. Monitoring the Reactions of 1 and 3 by ^{1}H NMR

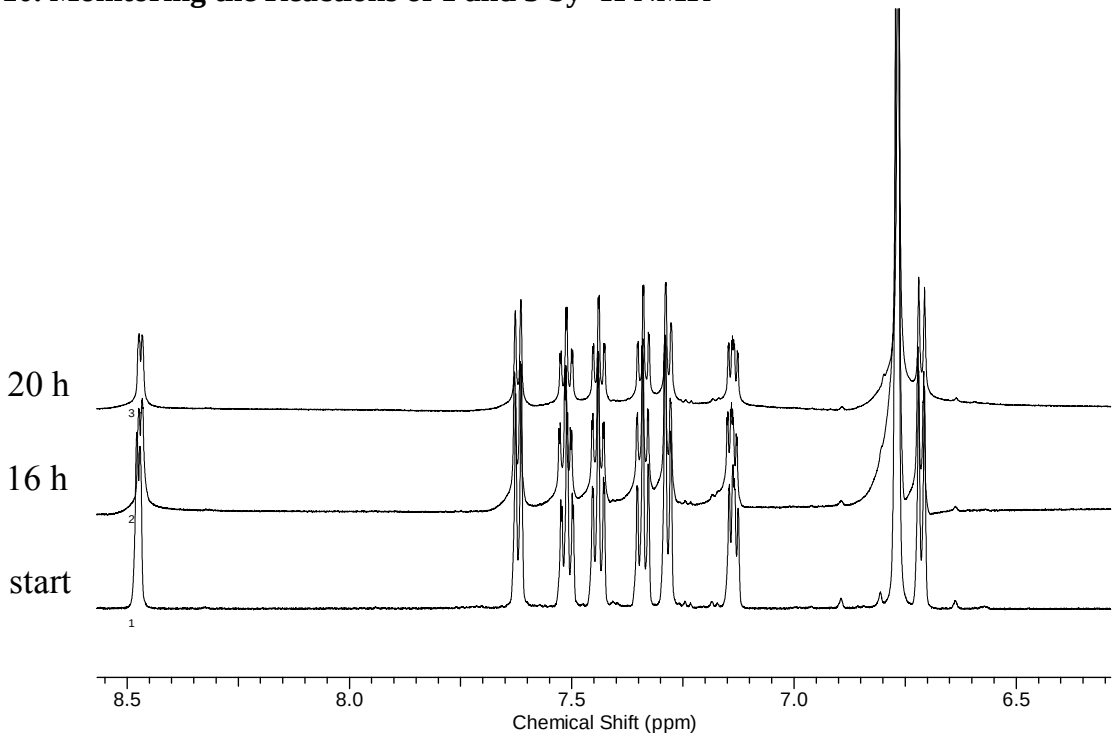


Figure S10. ^{1}H NMR spectra of **1** in CD_2Cl_2 showing that no reaction occurred after the addition of 10 eq. H_2O for 16 hrs and the subsequent addition of 1.5 eq. Et_3N for 4 hrs (16 h to 20 h) at ambient temperature.

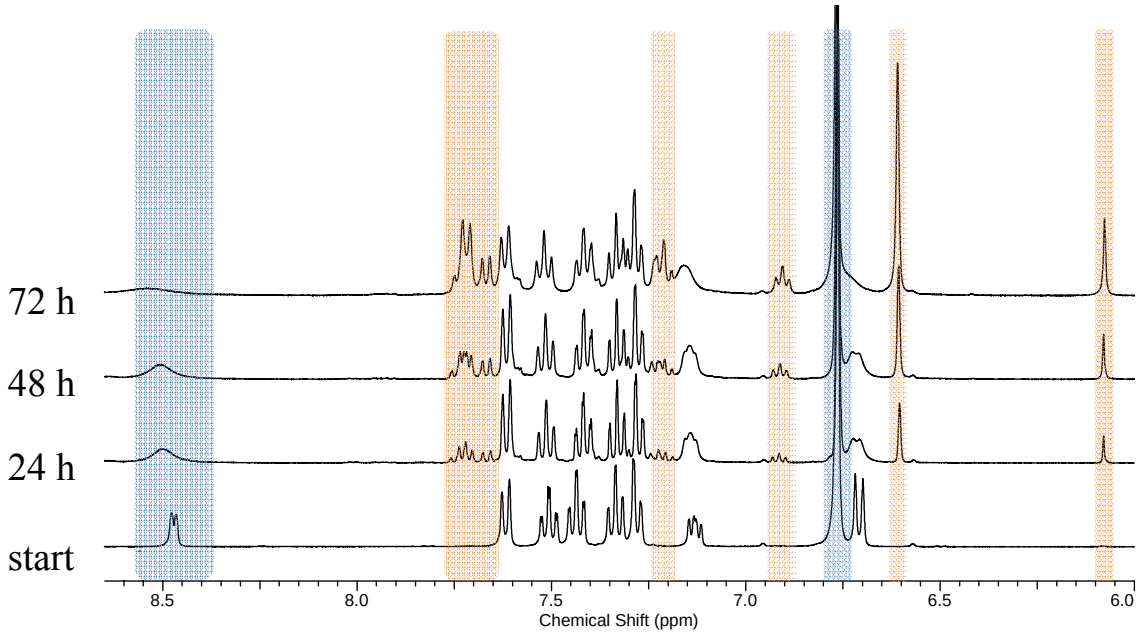


Figure S11. ^{1}H NMR spectra of **1** in CD_2Cl_2 showing the change after the addition of 10 eq. H_2O and 10 mol% CuI.

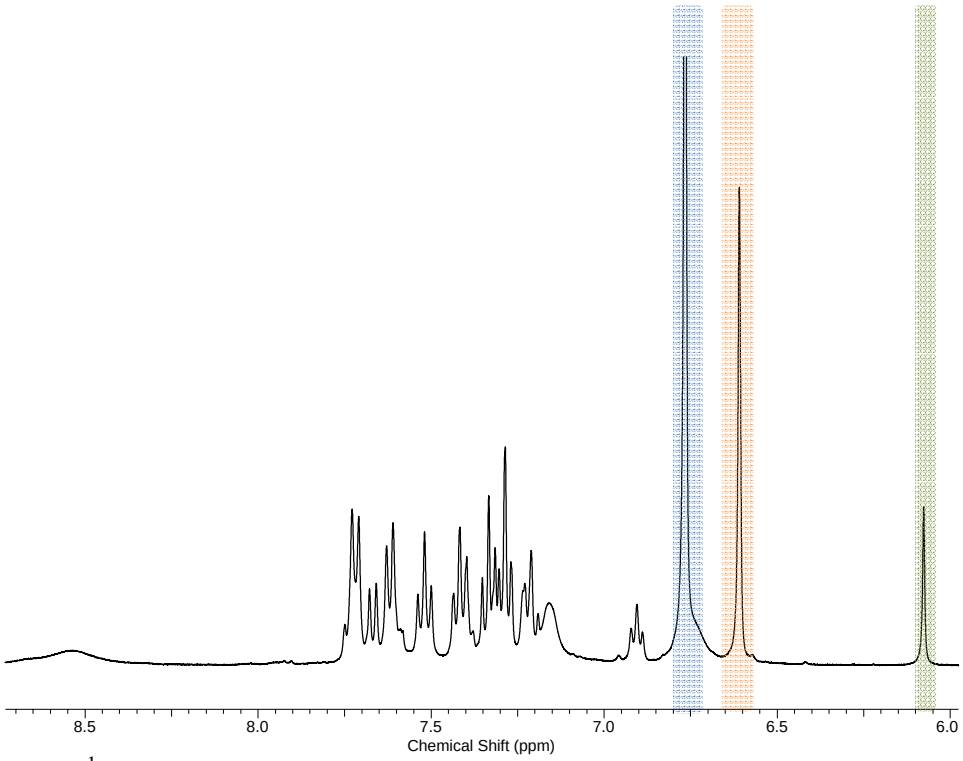


Figure S12a. ^{1}H NMR spectrum showing 40% conversion of **1** (highlighted by a representative peak in blue) to **2** (highlighted by a representative peak in orange) obtained using the condition described in the experimental section. Note the vinyl proton of **2** at 6.1 ppm (green).

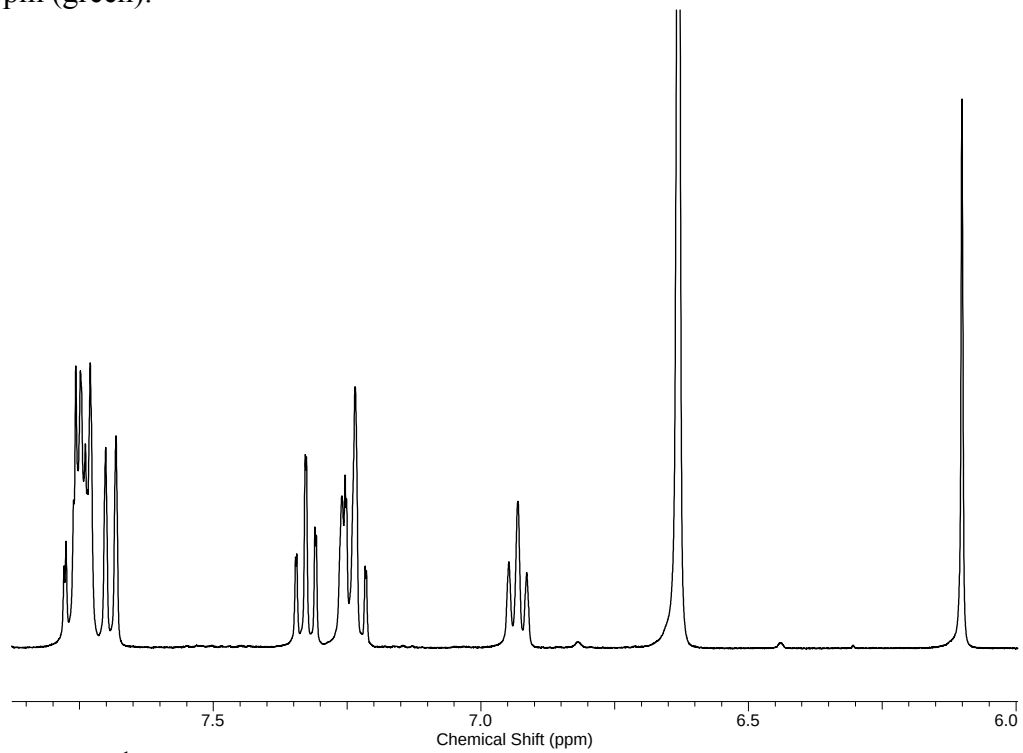


Figure S12b. ^{1}H NMR spectrum of the expanded aromatic region of **2** in CD_2Cl_2.

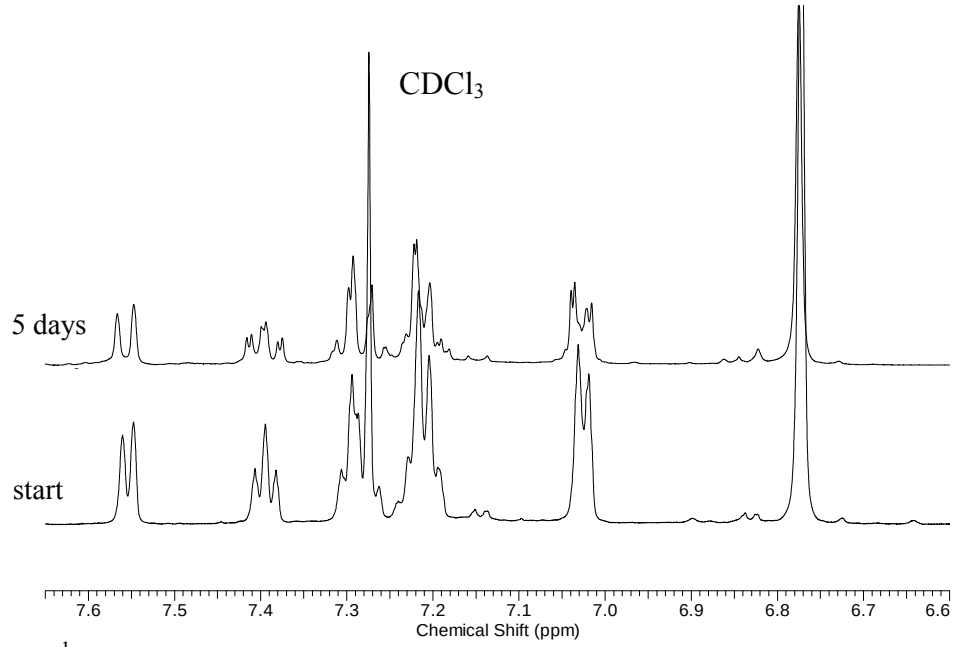


Figure S13. ^{1}H NMR spectra of **3** before and after being kept at ambient temperature for 5 days in $CDCl_3$ in the presence of 10% CuI, 10 eq. H_2O, and 10 eq. Et_3N. The top and bottom spectra were recorded using the 600 and 300 MHz NMR spectrometer, respectively.

S11. X-ray diffraction analysis

Single crystals of **1**, **2** and **3** were mounted on glass fibers for data collection. Data were collected on a Bruker Apex II single-crystal X-ray diffractometer with graphite-monochromated Mo Kα radiation, operated at 50 kV and 30 mA and at 180 K. Data were processed on a PC with the aid of the Bruker SHELXTL software package (version 6.14)[3] and corrected for absorption effects. No significant decay was observed. Compound **2** co-crystallized with a disordered diethylether molecule (0.5 diethylether per molecule of **2**), which was removed using the Platon Squeeze routine[4] to improve the overall quality of the structure.

References

1. Demas, N.J.; Crosby, G. A. *J. Am. Chem. Soc.,* **1970**, *29*, 7262.
2. Fukazawa, A.; Yamada, H.; Yamaguchi, S. *Angew. Chem. Int. Ed*., **2008**, *47*, 5582.
3. SHELXTL Version 6.14, Bruker AXS, 2000-2003.
4. Spek, A. L. Acta Crysl. **1990**, *A46*, C34.

Table 1. Crystal data and structure refinement for 1.

Identification code	louis21	
Empirical formula	C31 H30 B N	
Formula weight	427.37	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.148(12) Å	α= 90°.
	b = 23.74(3) Å	β= 92.161(16)°.
	c = 12.404(18) Å	γ = 90°.
Volume	2398(6) $Å^3$	
Z	4	
Density (calculated)	1.184 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	912	
Crystal size	0.10 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.38 to 26.00°.	
Index ranges	-9<=h<=10, -29<=k<=29, -15<=l<=15	
Reflections collected	16510	
Independent reflections	4640 [R(int) = 0.1592]	
Completeness to theta = 26.00°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9987 and 0.9933	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4640 / 0 / 305	
Goodness-of-fit on F^2	1.097	
Final R indices [I>2sigma(I)]	R1 = 0.1279, wR2 = 0.3261	
R indices (all data)	R1 = 0.2376, wR2 = 0.3848	
Extinction coefficient	0.026(6)	
Largest diff. peak and hole	0.411 and -0.386 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	9753(8)	2432(3)	6050(5)	63(2)
B(1)	8205(9)	4654(3)	7665(6)	47(2)
C(1)	7195(8)	4286(3)	8478(5)	46(2)
C(2)	6627(8)	4537(3)	9400(6)	54(2)
C(3)	5904(9)	4243(3)	10201(6)	59(2)
C(4)	5662(9)	3669(4)	10084(6)	61(2)
C(5)	6172(8)	3403(3)	9166(6)	53(2)
C(6)	6976(8)	3696(3)	8374(5)	46(2)
C(7)	7514(9)	3392(3)	7457(6)	53(2)
C(8)	7962(9)	3122(3)	6726(6)	51(2)
C(9)	8661(9)	2839(3)	5813(6)	54(2)
C(10)	8244(9)	3009(3)	4788(6)	57(2)
C(11)	8995(10)	2770(3)	3945(6)	64(2)
C(12)	10141(10)	2346(3)	4154(7)	69(2)
C(13)	10466(10)	2212(4)	5206(6)	68(2)
C(14)	7644(8)	5277(3)	7466(5)	48(2)
C(15)	8677(8)	5740(3)	7657(5)	49(2)
C(16)	8098(9)	6283(3)	7564(5)	55(2)
C(17)	6474(9)	6415(3)	7271(6)	56(2)
C(18)	5464(9)	5954(3)	7035(6)	55(2)
C(19)	5968(9)	5406(3)	7127(5)	50(2)
C(20)	4760(9)	4944(3)	6854(6)	66(2)
C(21)	5900(10)	7001(3)	7195(6)	69(2)
C(22)	10471(9)	5668(3)	8004(6)	61(2)
C(23)	9726(8)	4376(3)	7177(5)	46(2)
C(24)	11017(8)	4135(3)	7833(5)	47(2)
C(25)	12238(8)	3839(3)	7344(6)	49(2)
C(28)	9813(8)	4313(3)	6051(5)	49(2)
C(26)	12290(8)	3764(3)	6261(6)	52(2)
C(27)	11060(9)	4008(3)	5633(6)	54(2)
C(31)	8434(9)	4531(3)	5281(6)	55(2)

C(30)	13628(10)	3428(3)	5754(7)	71(2)
C(29)	11057(9)	4198(3)	9038(5)	58(2)

Table 3. Bond lengths [Å] and angles [°] for 1.

N(1)-C(13)	1.324(9)	C(16)-H(16A)	0.9500
N(1)-C(9)	1.340(9)	C(17)-C(18)	1.394(10)
B(1)-C(23)	1.547(10)	C(17)-C(21)	1.468(10)
B(1)-C(14)	1.563(11)	C(18)-C(19)	1.368(9)
B(1)-C(1)	1.588(11)	C(18)-H(18A)	0.9500
C(1)-C(2)	1.386(9)	C(19)-C(20)	1.503(10)
C(1)-C(6)	1.416(10)	C(20)-H(20A)	0.9800
C(2)-C(3)	1.366(10)	C(20)-H(20B)	0.9800
C(2)-H(2A)	0.9500	C(20)-H(20C)	0.9800
C(3)-C(4)	1.384(11)	C(21)-H(21A)	0.9800
C(3)-H(3A)	0.9500	C(21)-H(21B)	0.9800
C(4)-C(5)	1.380(10)	C(21)-H(21C)	0.9800
C(4)-H(4A)	0.9500	C(22)-H(22A)	0.9800
C(5)-C(6)	1.388(9)	C(22)-H(22B)	0.9800
C(5)-H(5A)	0.9500	C(22)-H(22C)	0.9800
C(6)-C(7)	1.430(10)	C(23)-C(28)	1.410(9)
C(7)-C(8)	1.178(9)	C(23)-C(24)	1.425(9)
C(8)-C(9)	1.452(10)	C(24)-C(25)	1.378(9)
C(9)-C(10)	1.364(10)	C(24)-C(29)	1.501(9)
C(10)-C(11)	1.355(10)	C(25)-C(26)	1.358(9)
C(10)-H(10A)	0.9500	C(25)-H(25A)	0.9500
C(11)-C(12)	1.391(11)	C(28)-C(27)	1.366(9)
C(11)-H(11A)	0.9500	C(28)-C(31)	1.536(9)
C(12)-C(13)	1.359(11)	C(26)-C(27)	1.374(10)
C(12)-H(12A)	0.9500	C(26)-C(30)	1.506(10)
C(13)-H(13A)	0.9500	C(27)-H(27A)	0.9500
C(14)-C(15)	1.400(9)	C(31)-H(31A)	0.9800
C(14)-C(19)	1.447(9)	C(31)-H(31B)	0.9800
C(15)-C(16)	1.377(10)	C(31)-H(31C)	0.9800
C(15)-C(22)	1.518(10)	C(30)-H(30A)	0.9800
C(16)-C(17)	1.395(10)	C(30)-H(30B)	0.9800

C(30)-H(30C)	0.9800	C(10)-C(11)-H(11A)	120.7
C(29)-H(29A)	0.9800	C(12)-C(11)-H(11A)	120.7
C(29)-H(29B)	0.9800	C(13)-C(12)-C(11)	117.0(7)
C(29)-H(29C)	0.9800	C(13)-C(12)-H(12A)	121.5
		C(11)-C(12)-H(12A)	121.5
C(13)-N(1)-C(9)	114.8(6)	N(1)-C(13)-C(12)	126.2(8)
C(23)-B(1)-C(14)	125.1(6)	N(1)-C(13)-H(13A)	116.9
C(23)-B(1)-C(1)	117.1(6)	C(12)-C(13)-H(13A)	116.9
C(14)-B(1)-C(1)	117.7(6)	C(15)-C(14)-C(19)	115.9(6)
C(2)-C(1)-C(6)	117.1(6)	C(15)-C(14)-B(1)	123.1(6)
C(2)-C(1)-B(1)	119.0(6)	C(19)-C(14)-B(1)	120.9(6)
C(6)-C(1)-B(1)	123.6(6)	C(16)-C(15)-C(14)	121.3(6)
C(3)-C(2)-C(1)	123.2(7)	C(16)-C(15)-C(22)	116.9(6)
C(3)-C(2)-H(2A)	118.4	C(14)-C(15)-C(22)	121.7(6)
C(1)-C(2)-H(2A)	118.4	C(15)-C(16)-C(17)	123.4(7)
C(2)-C(3)-C(4)	119.4(7)	C(15)-C(16)-H(16A)	118.3
C(2)-C(3)-H(3A)	120.3	C(17)-C(16)-H(16A)	118.3
C(4)-C(3)-H(3A)	120.3	C(18)-C(17)-C(16)	115.2(7)
C(5)-C(4)-C(3)	119.4(7)	C(18)-C(17)-C(21)	123.1(7)
C(5)-C(4)-H(4A)	120.3	C(16)-C(17)-C(21)	121.7(7)
C(3)-C(4)-H(4A)	120.3	C(19)-C(18)-C(17)	123.8(7)
C(4)-C(5)-C(6)	121.3(7)	C(19)-C(18)-H(18A)	118.1
C(4)-C(5)-H(5A)	119.3	C(17)-C(18)-H(18A)	118.1
C(6)-C(5)-H(5A)	119.3	C(18)-C(19)-C(14)	120.2(6)
C(5)-C(6)-C(1)	119.5(6)	C(18)-C(19)-C(20)	118.9(6)
C(5)-C(6)-C(7)	118.4(6)	C(14)-C(19)-C(20)	120.9(6)
C(1)-C(6)-C(7)	122.1(6)	C(19)-C(20)-H(20A)	109.5
C(8)-C(7)-C(6)	177.5(7)	C(19)-C(20)-H(20B)	109.5
C(7)-C(8)-C(9)	173.4(8)	H(20A)-C(20)-H(20B)	109.5
N(1)-C(9)-C(10)	123.9(7)	C(19)-C(20)-H(20C)	109.5
N(1)-C(9)-C(8)	116.1(6)	H(20A)-C(20)-H(20C)	109.5
C(10)-C(9)-C(8)	120.0(7)	H(20B)-C(20)-H(20C)	109.5
C(11)-C(10)-C(9)	119.4(7)	C(17)-C(21)-H(21A)	109.5
C(11)-C(10)-H(10A)	120.3	C(17)-C(21)-H(21B)	109.5
C(9)-C(10)-H(10A)	120.3	H(21A)-C(21)-H(21B)	109.5
C(10)-C(11)-C(12)	118.6(7)	C(17)-C(21)-H(21C)	109.5

H(21A)-C(21)-H(21C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(15)-C(22)-H(22A)	109.5	C(24)-C(29)-H(29A)	109.5
C(15)-C(22)-H(22B)	109.5	C(24)-C(29)-H(29B)	109.5
H(22A)-C(22)-H(22B)	109.5	H(29A)-C(29)-H(29B)	109.5
C(15)-C(22)-H(22C)	109.5	C(24)-C(29)-H(29C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(28)-C(23)-C(24)	117.3(6)		
C(28)-C(23)-B(1)	120.2(6)		
C(24)-C(23)-B(1)	122.2(6)		
C(25)-C(24)-C(23)	118.9(6)		
C(25)-C(24)-C(29)	120.0(6)		
C(23)-C(24)-C(29)	121.1(6)		
C(26)-C(25)-C(24)	123.6(6)		
C(26)-C(25)-H(25A)	118.2		
C(24)-C(25)-H(25A)	118.2		
C(27)-C(28)-C(23)	119.9(6)		
C(27)-C(28)-C(31)	118.7(6)		
C(23)-C(28)-C(31)	121.1(6)		
C(25)-C(26)-C(27)	117.1(7)		
C(25)-C(26)-C(30)	122.2(7)		
C(27)-C(26)-C(30)	120.7(7)		
C(28)-C(27)-C(26)	123.2(7)		
C(28)-C(27)-H(27A)	118.4		
C(26)-C(27)-H(27A)	118.4		
C(28)-C(31)-H(31A)	109.5		
C(28)-C(31)-H(31B)	109.5		
H(31A)-C(31)-H(31B)	109.5		
C(28)-C(31)-H(31C)	109.5		
H(31A)-C(31)-H(31C)	109.5		
H(31B)-C(31)-H(31C)	109.5		
C(26)-C(30)-H(30A)	109.5		
C(26)-C(30)-H(30B)	109.5		
H(30A)-C(30)-H(30B)	109.5		
C(26)-C(30)-H(30C)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

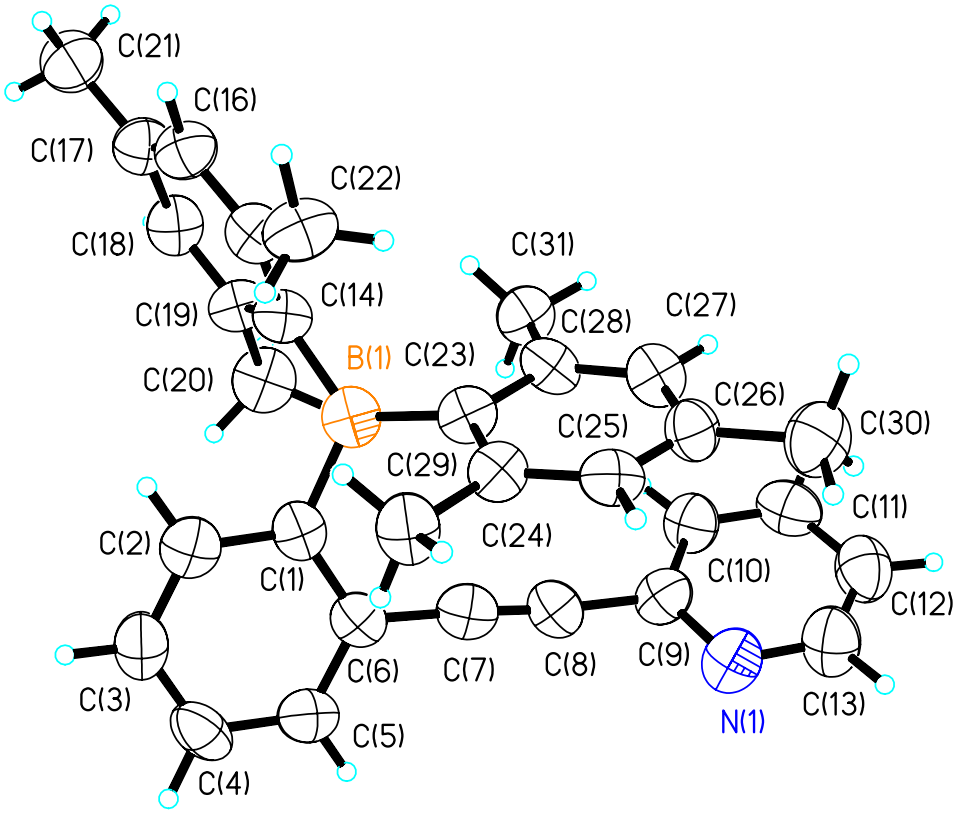
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	64(4)	64(4)	59(4)	-7(3)	-10(3)	6(3)
B(1)	34(5)	62(5)	44(4)	-4(4)	-14(3)	-4(4)
C(1)	34(4)	61(5)	43(4)	-1(3)	-6(3)	4(3)
C(2)	45(4)	63(4)	52(4)	2(4)	-13(3)	7(3)
C(3)	57(5)	72(5)	47(4)	-6(4)	-6(4)	19(4)
C(4)	52(5)	86(6)	44(4)	19(4)	5(4)	13(4)
C(5)	41(4)	55(4)	63(5)	9(4)	-2(4)	-1(3)
C(6)	39(4)	58(4)	40(4)	3(3)	-10(3)	2(3)
C(7)	45(4)	62(5)	51(5)	6(4)	-10(4)	-2(3)
C(8)	46(4)	65(5)	43(4)	-1(4)	-3(3)	-3(4)
C(9)	60(5)	50(4)	52(4)	-4(3)	-8(4)	1(4)
C(10)	61(5)	61(5)	49(5)	-10(4)	-5(4)	-2(4)
C(11)	71(6)	71(5)	50(5)	3(4)	-5(4)	-16(4)
C(12)	63(6)	73(5)	71(6)	-15(4)	10(4)	-7(4)
C(13)	68(6)	86(6)	50(5)	-9(4)	-7(4)	14(4)
C(14)	39(4)	52(4)	51(4)	5(3)	-5(3)	-3(3)
C(15)	45(4)	60(5)	42(4)	-1(3)	-10(3)	-3(3)
C(16)	58(5)	51(4)	56(4)	-1(3)	-6(4)	-3(4)
C(17)	53(5)	57(5)	57(4)	4(3)	-2(4)	4(4)
C(18)	47(4)	63(5)	53(4)	0(3)	-7(3)	8(4)
C(19)	46(4)	48(4)	55(4)	4(3)	-10(3)	-4(3)
C(20)	50(5)	78(5)	68(5)	-3(4)	-15(4)	0(4)
C(21)	72(6)	65(5)	70(5)	5(4)	5(4)	7(4)
C(22)	47(5)	56(4)	79(5)	4(4)	-14(4)	-7(3)
C(23)	41(4)	51(4)	44(4)	-2(3)	-12(3)	-4(3)
C(24)	34(4)	52(4)	54(4)	-3(3)	-6(3)	-3(3)
C(25)	36(4)	54(4)	56(5)	8(3)	-6(3)	-5(3)
C(28)	37(4)	67(4)	41(4)	8(3)	-4(3)	-4(3)
C(26)	40(4)	61(4)	56(5)	-1(3)	6(3)	3(3)
C(27)	42(4)	68(5)	50(4)	-4(4)	-5(3)	-4(4)

C(31)	44(4)	63(4)	56(4)	4(3)	-8(3)	8(3)
C(30)	52(5)	79(5)	83(6)	-1(5)	-2(4)	9(4)
C(29)	51(5)	74(5)	49(4)	-1(4)	-8(3)	10(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	6745	4933	9480	64
H(3A)	5571	4431	10833	71
H(4A)	5149	3460	10631	73
H(5A)	5969	3012	9074	64
H(10A)	7435	3292	4666	69
H(11A)	8744	2890	3227	77
H(12A)	10673	2158	3587	83
H(13A)	11284	1933	5349	82
H(16A)	8844	6584	7708	66
H(18A)	4362	6025	6796	66
H(20A)	3976	5075	6290	99
H(20B)	4168	4843	7499	99
H(20C)	5349	4614	6595	99
H(21A)	4839	7034	7536	104
H(21B)	5777	7110	6434	104
H(21C)	6702	7248	7565	104
H(22A)	11026	6034	7985	92
H(22B)	10996	5407	7512	92
H(22C)	10550	5517	8739	92
H(25A)	13091	3680	7788	58
H(27A)	11078	3963	4873	64
H(31A)	8772	4495	4534	82
H(31B)	8214	4928	5440	82
H(31C)	7436	4309	5378	82
H(30A)	14298	3241	6320	107
H(30B)	14322	3681	5344	107
H(30C)	13135	3145	5268	107

H(29A)	12138	4085	9336	87
H(29B)	10209	3959	9340	87
H(29C)	10851	4592	9225	87



A diagram showing the molecular structure of compound **1** with labelling schemes and 50% thermal ellipsoids.

Table 1. Crystal data and structure refinement for 2.

Identification code	louis20	
Empirical formula	C31 H32 B N O	
Formula weight	445.39	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.196(15) Å	α= 90°.
	b = 13.291(15) Å	β= 98.526(13)°.
	c = 15.960(18) Å	γ = 90°.
Volume	2768(5) $Å^3$	
Z	4	
Density (calculated)	1.069 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	952	
Crystal size	0.05 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.19 to 26.00°.	
Index ranges	-16<=h<=16, -16<=k<=16, -19<=l<=19	
Reflections collected	25307	
Independent reflections	5443 [R(int) = 0.1889]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9969 and 0.9969	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5443 / 1 / 317	
Goodness-of-fit on F^2	0.915	
Final R indices [I>2sigma(I)]	R1 = 0.0982, wR2 = 0.2132	
R indices (all data)	R1 = 0.2209, wR2 = 0.2674	
Extinction coefficient	0.0035(12)	
Largest diff. peak and hole	0.278 and -0.385 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4496(3)	1304(3)	-4798(2)	44(1)
B(1)	3209(4)	1291(4)	-2557(3)	39(1)
O(1)	3932(3)	1348(2)	-3284(2)	43(1)
C(1)	4132(4)	1241(3)	-1769(3)	40(1)
C(2)	4166(4)	1271(3)	-871(3)	47(1)
C(3)	5090(4)	1259(3)	-338(3)	47(1)
C(4)	6015(4)	1300(3)	-649(3)	50(1)
C(5)	6010(4)	1315(3)	-1523(3)	42(1)
C(6)	5088(4)	1304(3)	-2046(3)	39(1)
C(7)	4919(4)	1324(3)	-2989(3)	40(1)
C(8)	5663(4)	1316(3)	-3487(3)	41(1)
C(9)	5466(4)	1273(3)	-4397(3)	42(1)
C(10)	6247(4)	1205(3)	-4900(3)	47(1)
C(11)	6000(4)	1148(3)	-5774(3)	47(1)
C(12)	5001(4)	1191(3)	-6146(3)	46(1)
C(13)	4232(4)	1272(3)	-5668(3)	49(1)
C(14)	2637(4)	2367(4)	-2470(3)	42(1)
C(15)	2875(4)	3315(4)	-2794(3)	44(1)
C(16)	2423(4)	4183(4)	-2570(3)	47(1)
C(17)	1696(4)	4204(4)	-2018(3)	48(1)
C(18)	1451(4)	3287(4)	-1713(3)	51(1)
C(19)	1876(4)	2401(4)	-1904(3)	46(1)
C(20)	1498(4)	1451(4)	-1546(3)	57(2)
C(21)	3645(4)	3447(4)	-3421(3)	55(2)
C(22)	1204(4)	5192(4)	-1799(4)	68(2)
C(23)	2527(4)	311(4)	-2875(3)	43(1)
C(24)	2597(4)	-655(4)	-2502(3)	50(1)
C(25)	2104(4)	-1490(4)	-2887(3)	53(1)
C(26)	1492(4)	-1416(4)	-3670(3)	51(1)
C(27)	1373(4)	-493(4)	-4019(3)	54(1)
C(28)	1848(4)	367(4)	-3668(3)	50(1)

C(29)	1645(4)	1354(4)	-4141(3)	62(2)
C(30)	3296(4)	-875(4)	-1655(3)	63(2)
C(31)	1046(4)	-2362(4)	-4102(4)	77(2)

Table 3. Bond lengths [Å] and angles [°] for 2.

N(1)-C(9)	1.344(6)	C(14)-C(15)	1.414(6)
N(1)-C(13)	1.381(6)	C(14)-C(19)	1.448(7)
N(1)-H(1A)	0.98(3)	C(15)-C(16)	1.370(6)
B(1)-O(1)	1.609(6)	C(15)-C(21)	1.539(7)
B(1)-C(1)	1.617(7)	C(16)-C(17)	1.396(7)
B(1)-C(23)	1.621(7)	C(16)-H(16A)	0.9500
B(1)-C(14)	1.632(7)	C(17)-C(18)	1.369(7)
O(1)-C(7)	1.318(5)	C(17)-C(22)	1.528(7)
C(1)-C(6)	1.400(6)	C(18)-C(19)	1.358(6)
C(1)-C(2)	1.427(6)	C(18)-H(18A)	0.9500
C(2)-C(3)	1.380(6)	C(19)-C(20)	1.501(7)
C(2)-H(2A)	0.9500	C(20)-H(20A)	0.9800
C(3)-C(4)	1.385(7)	C(20)-H(20B)	0.9800
C(3)-H(3A)	0.9500	C(20)-H(20C)	0.9800
C(4)-C(5)	1.395(6)	C(21)-H(21A)	0.9800
C(4)-H(4A)	0.9500	C(21)-H(21B)	0.9800
C(5)-C(6)	1.370(6)	C(21)-H(21C)	0.9800
C(5)-H(5A)	0.9500	C(22)-H(22A)	0.9800
C(6)-C(7)	1.489(6)	C(22)-H(22B)	0.9800
C(7)-C(8)	1.352(6)	C(22)-H(22C)	0.9800
C(8)-C(9)	1.438(6)	C(23)-C(24)	1.413(7)
C(8)-H(8A)	0.9500	C(23)-C(28)	1.440(6)
C(9)-C(10)	1.399(6)	C(24)-C(25)	1.384(7)
C(10)-C(11)	1.386(6)	C(24)-C(30)	1.547(7)
C(10)-H(10A)	0.9500	C(25)-C(26)	1.387(7)
C(11)-C(12)	1.365(6)	C(25)-H(25A)	0.9500
C(11)-H(11A)	0.9500	C(26)-C(27)	1.347(7)
C(12)-C(13)	1.362(7)	C(26)-C(31)	1.510(7)
C(12)-H(12A)	0.9500	C(27)-C(28)	1.382(7)
C(13)-H(13A)	0.9500	C(27)-H(27A)	0.9500

C(28)-C(29)	1.517(7)	C(5)-C(6)-C(1)	124.7(4)
C(29)-H(29A)	0.9800	C(5)-C(6)-C(7)	127.0(4)
C(29)-H(29B)	0.9800	C(1)-C(6)-C(7)	108.3(4)
C(29)-H(29C)	0.9800	O(1)-C(7)-C(8)	123.8(4)
C(30)-H(30A)	0.9800	O(1)-C(7)-C(6)	110.7(4)
C(30)-H(30B)	0.9800	C(8)-C(7)-C(6)	125.5(5)
C(30)-H(30C)	0.9800	C(7)-C(8)-C(9)	123.8(5)
C(31)-H(31A)	0.9800	C(7)-C(8)-H(8A)	118.1
C(31)-H(31B)	0.9800	C(9)-C(8)-H(8A)	118.1
C(31)-H(31C)	0.9800	N(1)-C(9)-C(10)	117.4(4)
		N(1)-C(9)-C(8)	119.7(4)
C(9)-N(1)-C(13)	123.9(4)	C(10)-C(9)-C(8)	122.9(5)
C(9)-N(1)-H(1A)	127(3)	C(11)-C(10)-C(9)	119.8(5)
C(13)-N(1)-H(1A)	109(3)	C(11)-C(10)-H(10A)	120.1
O(1)-B(1)-C(1)	96.0(4)	C(9)-C(10)-H(10A)	120.1
O(1)-B(1)-C(23)	99.9(3)	C(12)-C(11)-C(10)	120.2(4)
C(1)-B(1)-C(23)	122.0(4)	C(12)-C(11)-H(11A)	119.9
O(1)-B(1)-C(14)	110.5(4)	C(10)-C(11)-H(11A)	119.9
C(1)-B(1)-C(14)	105.9(4)	C(13)-C(12)-C(11)	120.7(5)
C(23)-B(1)-C(14)	119.3(4)	C(13)-C(12)-H(12A)	119.6
C(7)-O(1)-B(1)	113.7(3)	C(11)-C(12)-H(12A)	119.6
C(6)-C(1)-C(2)	114.8(4)	C(12)-C(13)-N(1)	117.9(5)
C(6)-C(1)-B(1)	111.2(4)	C(12)-C(13)-H(13A)	121.0
C(2)-C(1)-B(1)	133.5(4)	N(1)-C(13)-H(13A)	121.0
C(3)-C(2)-C(1)	120.8(5)	C(15)-C(14)-C(19)	114.3(4)
C(3)-C(2)-H(2A)	119.6	C(15)-C(14)-B(1)	128.3(4)
C(1)-C(2)-H(2A)	119.6	C(19)-C(14)-B(1)	116.9(4)
C(2)-C(3)-C(4)	121.6(4)	C(16)-C(15)-C(14)	121.8(5)
C(2)-C(3)-H(3A)	119.2	C(16)-C(15)-C(21)	115.3(4)
C(4)-C(3)-H(3A)	119.2	C(14)-C(15)-C(21)	122.9(4)
C(3)-C(4)-C(5)	119.0(5)	C(15)-C(16)-C(17)	123.2(5)
C(3)-C(4)-H(4A)	120.5	C(15)-C(16)-H(16A)	118.4
C(5)-C(4)-H(4A)	120.5	C(17)-C(16)-H(16A)	118.4
C(6)-C(5)-C(4)	118.8(5)	C(18)-C(17)-C(16)	115.4(5)
C(6)-C(5)-H(5A)	120.6	C(18)-C(17)-C(22)	123.5(5)
C(4)-C(5)-H(5A)	120.6	C(16)-C(17)-C(22)	121.1(5)

C(19)-C(18)-C(17)	124.4(5)	C(26)-C(27)-C(28)	124.6(5)
C(19)-C(18)-H(18A)	117.8	C(26)-C(27)-H(27A)	117.7
C(17)-C(18)-H(18A)	117.8	C(28)-C(27)-H(27A)	117.7
C(18)-C(19)-C(14)	121.0(4)	C(27)-C(28)-C(23)	119.9(5)
C(18)-C(19)-C(20)	118.2(5)	C(27)-C(28)-C(29)	118.5(5)
C(14)-C(19)-C(20)	120.7(4)	C(23)-C(28)-C(29)	121.5(5)
C(19)-C(20)-H(20A)	109.5	C(28)-C(29)-H(29A)	109.5
C(19)-C(20)-H(20B)	109.5	C(28)-C(29)-H(29B)	109.5
H(20A)-C(20)-H(20B)	109.5	H(29A)-C(29)-H(29B)	109.5
C(19)-C(20)-H(20C)	109.5	C(28)-C(29)-H(29C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(20B)-C(20)-H(20C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(15)-C(21)-H(21A)	109.5	C(24)-C(30)-H(30A)	109.5
C(15)-C(21)-H(21B)	109.5	C(24)-C(30)-H(30B)	109.5
H(21A)-C(21)-H(21B)	109.5	H(30A)-C(30)-H(30B)	109.5
C(15)-C(21)-H(21C)	109.5	C(24)-C(30)-H(30C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(17)-C(22)-H(22A)	109.5	C(26)-C(31)-H(31A)	109.5
C(17)-C(22)-H(22B)	109.5	C(26)-C(31)-H(31B)	109.5
H(22A)-C(22)-H(22B)	109.5	H(31A)-C(31)-H(31B)	109.5
C(17)-C(22)-H(22C)	109.5	C(26)-C(31)-H(31C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(31A)-C(31)-H(31C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(24)-C(23)-C(28)	114.3(4)		
C(24)-C(23)-B(1)	126.9(4)		
C(28)-C(23)-B(1)	118.5(4)		
C(25)-C(24)-C(23)	123.0(5)		
C(25)-C(24)-C(30)	114.6(5)		
C(23)-C(24)-C(30)	122.2(4)		
C(24)-C(25)-C(26)	121.0(5)		
C(24)-C(25)-H(25A)	119.5		
C(26)-C(25)-H(25A)	119.5		
C(27)-C(26)-C(25)	117.0(5)		
C(27)-C(26)-C(31)	123.7(5)		
C(25)-C(26)-C(31)	119.2(5)		

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	57(3)	49(3)	25(2)	0(2)	10(2)	0(2)
B(1)	55(4)	47(3)	17(2)	9(2)	10(2)	3(3)
O(1)	55(2)	59(2)	17(2)	0(1)	12(2)	2(2)
C(1)	62(3)	33(3)	27(2)	-3(2)	9(2)	2(2)
C(2)	75(4)	48(3)	21(2)	2(2)	16(3)	9(3)
C(3)	72(4)	47(3)	22(3)	4(2)	4(3)	-3(3)
C(4)	71(4)	49(3)	26(3)	1(2)	-4(3)	-3(3)
C(5)	57(3)	45(3)	24(2)	0(2)	7(2)	5(2)
C(6)	53(3)	37(3)	26(2)	3(2)	7(2)	4(2)
C(7)	56(3)	42(3)	24(2)	-3(2)	12(2)	0(3)
C(8)	54(3)	44(3)	25(2)	-2(2)	7(2)	-4(2)
C(9)	52(3)	41(3)	35(3)	2(2)	9(2)	-3(2)
C(10)	52(3)	59(3)	33(3)	5(2)	10(2)	4(3)
C(11)	60(4)	55(3)	30(3)	0(2)	21(3)	2(3)
C(12)	71(4)	48(3)	19(2)	-7(2)	9(3)	-2(3)
C(13)	65(4)	54(3)	26(3)	9(2)	2(2)	-5(3)
C(14)	50(3)	55(3)	18(2)	0(2)	1(2)	-8(2)
C(15)	58(3)	47(3)	25(3)	3(2)	3(2)	-8(3)
C(16)	65(4)	41(3)	33(3)	4(2)	2(3)	6(3)
C(17)	57(3)	58(4)	31(3)	-6(3)	8(2)	7(3)
C(18)	63(4)	60(4)	30(3)	6(3)	15(2)	2(3)
C(19)	63(3)	45(3)	30(3)	6(2)	9(2)	5(3)
C(20)	71(4)	65(4)	41(3)	0(3)	24(3)	1(3)
C(21)	84(4)	45(3)	41(3)	1(2)	28(3)	1(3)
C(22)	77(4)	78(4)	51(4)	-3(3)	16(3)	14(3)
C(23)	56(3)	53(3)	21(3)	-1(2)	11(2)	3(3)
C(24)	70(4)	51(3)	34(3)	-6(3)	23(3)	-4(3)
C(25)	63(4)	54(4)	45(3)	-8(3)	19(3)	-2(3)
C(26)	62(4)	51(4)	43(3)	-16(3)	16(3)	-11(3)
C(27)	55(4)	65(4)	41(3)	-9(3)	8(3)	-2(3)

C(28)	55(3)	60(4)	35(3)	-4(3)	6(3)	-1(3)
C(29)	73(4)	74(4)	34(3)	2(3)	-6(3)	1(3)
C(30)	109(5)	56(3)	23(3)	8(2)	9(3)	6(3)
C(31)	70(4)	88(5)	74(5)	-18(4)	14(3)	-9(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2.

	x	y	z	U(eq)
H(1A)	3870(30)	1340(30)	-4530(30)	52
H(2A)	3545	1299	-638	57
H(3A)	5092	1223	257	57
H(4A)	6644	1318	-272	60
H(5A)	6635	1332	-1752	50
H(8A)	6356	1339	-3221	49
H(10A)	6944	1199	-4644	57
H(11A)	6529	1077	-6114	56
H(12A)	4840	1164	-6746	55
H(13A)	3535	1305	-5924	59
H(16A)	2614	4801	-2802	56
H(18A)	951	3270	-1342	61
H(20A)	1251	1601	-1010	86
H(20B)	2060	963	-1445	86
H(20C)	938	1169	-1949	86
H(21A)	3762	4166	-3505	82
H(21B)	3369	3137	-3964	82
H(21C)	4294	3123	-3193	82
H(22A)	1365	5314	-1188	102
H(22B)	459	5149	-1961	102
H(22C)	1472	5745	-2108	102
H(25A)	2186	-2125	-2611	63
H(27A)	932	-429	-4544	64
H(29A)	1291	1222	-4714	92
H(29B)	2298	1693	-4175	92

H(29C)	1217	1785	-3840	92
H(30A)	3288	-1598	-1536	94
H(30B)	3045	-504	-1197	94
H(30C)	3998	-663	-1697	94
H(31A)	425	-2193	-4493	116
H(31B)	874	-2837	-3675	116
H(31C)	1549	-2669	-4417	116

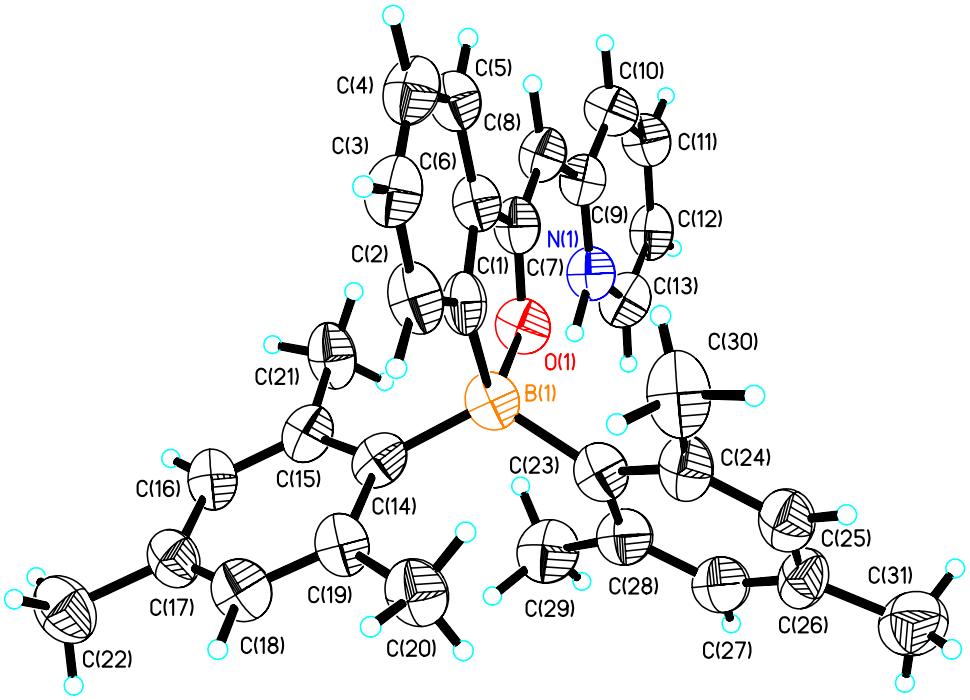


Table 1. Crystal data and structure refinement for compound 3.

Identification code	louis25	
Empirical formula	C32 H31 B	
Formula weight	426.38	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3686(14) Å	α= 65.465(2)°.
	b = 12.1651(18) Å	β= 81.937(2)°.
	c = 12.2768(18) Å	γ = 81.928(2)°.
Volume	1255.0(3) $Å^3$	
Z	2	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	456	
Crystal size	0.20 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.83 to 27.00°.	
Index ranges	-11<=h<=11, -15<=k<=15, -15<=l<=15	
Reflections collected	13712	
Independent reflections	5366 [R(int) = 0.0235]	
Completeness to theta = 27.00°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9969 and 0.9876	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5366 / 0 / 303	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1217	
R indices (all data)	R1 = 0.0629, wR2 = 0.1352	
Largest diff. peak and hole	0.244 and -0.179 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(22)	7363(2)	626(2)	-1420(2)	64(1)
C(18)	7460(2)	1207(1)	-566(1)	44(1)
C(19)	6317(2)	1236(1)	274(1)	39(1)
C(20)	6393(2)	1738(1)	1097(1)	34(1)
C(15)	7665(2)	2240(1)	1099(1)	33(1)
C(1)	9258(2)	2483(1)	2675(1)	34(1)
C(6)	10021(2)	1324(1)	3161(1)	35(1)
C(7)	9457(2)	271(1)	3196(1)	38(1)
C(8)	9030(2)	-631(1)	3241(1)	41(1)
C(9)	8549(2)	-1694(1)	3233(1)	38(1)
C(14)	7304(2)	-1618(1)	2692(2)	46(1)
C(13)	6872(2)	-2635(1)	2645(2)	47(1)
C(12)	7663(2)	-3744(1)	3134(1)	42(1)
C(31)	3160(2)	5904(2)	3407(2)	51(1)
C(27)	4343(2)	5100(1)	3061(1)	38(1)
C(26)	4987(2)	5463(1)	1890(1)	37(1)
C(25)	6093(2)	4739(1)	1555(1)	34(1)
C(30)	6785(2)	5213(1)	276(1)	43(1)
C(24)	6586(2)	3602(1)	2415(1)	33(1)
C(2)	9868(2)	3454(1)	2707(2)	43(1)
C(3)	11198(2)	3308(2)	3143(2)	50(1)
C(4)	11922(2)	2168(2)	3619(2)	49(1)
C(5)	11338(2)	1179(2)	3642(1)	45(1)
C(10)	9340(2)	-2822(1)	3731(1)	40(1)
C(11)	8896(2)	-3830(1)	3672(1)	42(1)
C(17)	8689(2)	1726(2)	-586(1)	46(1)
C(16)	8815(2)	2244(1)	212(1)	39(1)
C(21)	10189(2)	2838(2)	54(2)	54(1)
C(23)	5106(2)	1651(2)	2011(2)	44(1)
C(29)	5951(2)	3243(1)	3612(1)	35(1)
C(28)	4842(2)	3986(1)	3909(1)	38(1)

C(32)	6430(2)	2042(1)	4589(1)	49(1)
B(1)	7815(2)	2756(1)	2055(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for compound 3.

C(22)-C(18)	1.507(2)	C(27)-C(28)	1.387(2)
C(22)-H(22A)	0.9800	C(27)-C(26)	1.389(2)
C(22)-H(22B)	0.9800	C(26)-C(25)	1.395(2)
C(22)-H(22C)	0.9800	C(26)-H(26A)	0.9500
C(18)-C(17)	1.381(2)	C(25)-C(24)	1.4087(19)
C(18)-C(19)	1.386(2)	C(25)-C(30)	1.512(2)
C(19)-C(20)	1.394(2)	C(30)-H(30A)	0.9800
C(19)-H(19A)	0.9500	C(30)-H(30B)	0.9800
C(20)-C(15)	1.413(2)	C(30)-H(30C)	0.9800
C(20)-C(23)	1.511(2)	C(24)-C(29)	1.4147(19)
C(15)-C(16)	1.4193(19)	C(24)-B(1)	1.574(2)
C(15)-B(1)	1.574(2)	C(2)-C(3)	1.384(2)
C(1)-C(2)	1.399(2)	C(2)-H(2A)	0.9500
C(1)-C(6)	1.4119(19)	C(3)-C(4)	1.378(2)
C(1)-B(1)	1.571(2)	C(3)-H(3A)	0.9500
C(6)-C(5)	1.400(2)	C(4)-C(5)	1.379(2)
C(6)-C(7)	1.436(2)	C(4)-H(4A)	0.9500
C(7)-C(8)	1.196(2)	C(5)-H(5A)	0.9500
C(8)-C(9)	1.433(2)	C(10)-C(11)	1.381(2)
C(9)-C(14)	1.395(2)	C(10)-H(10A)	0.9500
C(9)-C(10)	1.396(2)	C(11)-H(11A)	0.9500
C(14)-C(13)	1.380(2)	C(17)-C(16)	1.392(2)
C(14)-H(14A)	0.9500	C(17)-H(17A)	0.9500
C(13)-C(12)	1.378(2)	C(16)-C(21)	1.514(2)
C(13)-H(13A)	0.9500	C(21)-H(21A)	0.9800
C(12)-C(11)	1.380(2)	C(21)-H(21B)	0.9800
C(12)-H(12A)	0.9500	C(21)-H(21C)	0.9800
C(31)-C(27)	1.508(2)	C(23)-H(23A)	0.9800
C(31)-H(31A)	0.9800	C(23)-H(23B)	0.9800
C(31)-H(31B)	0.9800	C(23)-H(23C)	0.9800
C(31)-H(31C)	0.9800	C(29)-C(28)	1.390(2)

C(29)-C(32)	1.512(2)	C(13)-C(14)-H(14A)	119.7
C(28)-H(28A)	0.9500	C(9)-C(14)-H(14A)	119.7
C(32)-H(32A)	0.9800	C(12)-C(13)-C(14)	120.50(15)
C(32)-H(32B)	0.9800	C(12)-C(13)-H(13A)	119.8
C(32)-H(32C)	0.9800	C(14)-C(13)-H(13A)	119.8
		C(13)-C(12)-C(11)	119.45(14)
C(18)-C(22)-H(22A)	109.5	C(13)-C(12)-H(12A)	120.3
C(18)-C(22)-H(22B)	109.5	C(11)-C(12)-H(12A)	120.3
H(22A)-C(22)-H(22B)	109.5	C(27)-C(31)-H(31A)	109.5
C(18)-C(22)-H(22C)	109.5	C(27)-C(31)-H(31B)	109.5
H(22A)-C(22)-H(22C)	109.5	H(31A)-C(31)-H(31B)	109.5
H(22B)-C(22)-H(22C)	109.5	C(27)-C(31)-H(31C)	109.5
C(17)-C(18)-C(19)	117.54(14)	H(31A)-C(31)-H(31C)	109.5
C(17)-C(18)-C(22)	121.39(15)	H(31B)-C(31)-H(31C)	109.5
C(19)-C(18)-C(22)	121.07(15)	C(28)-C(27)-C(26)	118.02(13)
C(18)-C(19)-C(20)	122.23(14)	C(28)-C(27)-C(31)	120.95(14)
C(18)-C(19)-H(19A)	118.9	C(26)-C(27)-C(31)	121.02(14)
C(20)-C(19)-H(19A)	118.9	C(27)-C(26)-C(25)	121.87(13)
C(19)-C(20)-C(15)	120.28(13)	C(27)-C(26)-H(26A)	119.1
C(19)-C(20)-C(23)	117.07(13)	C(25)-C(26)-H(26A)	119.1
C(15)-C(20)-C(23)	122.55(13)	C(26)-C(25)-C(24)	120.01(13)
C(20)-C(15)-C(16)	117.29(13)	C(26)-C(25)-C(30)	119.01(13)
C(20)-C(15)-B(1)	121.59(12)	C(24)-C(25)-C(30)	120.95(13)
C(16)-C(15)-B(1)	121.12(12)	C(25)-C(30)-H(30A)	109.5
C(2)-C(1)-C(6)	117.31(13)	C(25)-C(30)-H(30B)	109.5
C(2)-C(1)-B(1)	118.37(13)	H(30A)-C(30)-H(30B)	109.5
C(6)-C(1)-B(1)	124.27(12)	C(25)-C(30)-H(30C)	109.5
C(5)-C(6)-C(1)	120.21(13)	H(30A)-C(30)-H(30C)	109.5
C(5)-C(6)-C(7)	118.63(13)	H(30B)-C(30)-H(30C)	109.5
C(1)-C(6)-C(7)	121.14(13)	C(25)-C(24)-C(29)	118.08(13)
C(8)-C(7)-C(6)	177.69(16)	C(25)-C(24)-B(1)	121.02(12)
C(7)-C(8)-C(9)	177.04(16)	C(29)-C(24)-B(1)	120.89(12)
C(14)-C(9)-C(10)	118.53(14)	C(3)-C(2)-C(1)	121.99(15)
C(14)-C(9)-C(8)	120.64(14)	C(3)-C(2)-H(2A)	119.0
C(10)-C(9)-C(8)	120.80(14)	C(1)-C(2)-H(2A)	119.0
C(13)-C(14)-C(9)	120.57(14)	C(4)-C(3)-C(2)	119.74(15)

C(4)-C(3)-H(3A)	120.1	C(27)-C(28)-H(28A)	119.1
C(2)-C(3)-H(3A)	120.1	C(29)-C(28)-H(28A)	119.1
C(3)-C(4)-C(5)	120.20(15)	C(29)-C(32)-H(32A)	109.5
C(3)-C(4)-H(4A)	119.9	C(29)-C(32)-H(32B)	109.5
C(5)-C(4)-H(4A)	119.9	H(32A)-C(32)-H(32B)	109.5
C(4)-C(5)-C(6)	120.46(15)	C(29)-C(32)-H(32C)	109.5
C(4)-C(5)-H(5A)	119.8	H(32A)-C(32)-H(32C)	109.5
C(6)-C(5)-H(5A)	119.8	H(32B)-C(32)-H(32C)	109.5
C(11)-C(10)-C(9)	120.18(15)	C(1)-B(1)-C(15)	120.67(12)
C(11)-C(10)-H(10A)	119.9	C(1)-B(1)-C(24)	116.09(12)
C(9)-C(10)-H(10A)	119.9	C(15)-B(1)-C(24)	123.20(12)
C(12)-C(11)-C(10)	120.76(14)		
C(12)-C(11)-H(11A)	119.6		
C(10)-C(11)-H(11A)	119.6		
C(18)-C(17)-C(16)	122.37(14)		
C(18)-C(17)-H(17A)	118.8		
C(16)-C(17)-H(17A)	118.8		
C(17)-C(16)-C(15)	120.23(13)		
C(17)-C(16)-C(21)	117.08(13)		
C(15)-C(16)-C(21)	122.65(13)		
C(16)-C(21)-H(21A)	109.5		
C(16)-C(21)-H(21B)	109.5		
H(21A)-C(21)-H(21B)	109.5		
C(16)-C(21)-H(21C)	109.5		
H(21A)-C(21)-H(21C)	109.5		
H(21B)-C(21)-H(21C)	109.5		
C(20)-C(23)-H(23A)	109.5		
C(20)-C(23)-H(23B)	109.5		
H(23A)-C(23)-H(23B)	109.5		
C(20)-C(23)-H(23C)	109.5		
H(23A)-C(23)-H(23C)	109.5		
H(23B)-C(23)-H(23C)	109.5		
C(28)-C(29)-C(24)	120.20(13)		
C(28)-C(29)-C(32)	118.50(13)		
C(24)-C(29)-C(32)	121.28(13)		
C(27)-C(28)-C(29)	121.80(14)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(22)	77(1)	71(1)	61(1)	-45(1)	9(1)	-19(1)
C(18)	56(1)	39(1)	40(1)	-21(1)	0(1)	-6(1)
C(19)	44(1)	35(1)	42(1)	-18(1)	-3(1)	-7(1)
C(20)	36(1)	30(1)	36(1)	-13(1)	-2(1)	-2(1)
C(15)	35(1)	30(1)	33(1)	-12(1)	-2(1)	-2(1)
C(1)	34(1)	35(1)	37(1)	-20(1)	1(1)	-4(1)
C(6)	35(1)	37(1)	36(1)	-18(1)	2(1)	-2(1)
C(7)	39(1)	34(1)	40(1)	-14(1)	0(1)	0(1)
C(8)	44(1)	34(1)	41(1)	-15(1)	1(1)	-1(1)
C(9)	43(1)	32(1)	36(1)	-14(1)	5(1)	-5(1)
C(14)	48(1)	32(1)	52(1)	-13(1)	-7(1)	3(1)
C(13)	45(1)	44(1)	52(1)	-18(1)	-9(1)	-3(1)
C(12)	47(1)	36(1)	44(1)	-19(1)	-1(1)	-6(1)
C(31)	44(1)	47(1)	64(1)	-29(1)	-5(1)	6(1)
C(27)	32(1)	38(1)	50(1)	-23(1)	-8(1)	-1(1)
C(26)	39(1)	31(1)	45(1)	-15(1)	-14(1)	-1(1)
C(25)	36(1)	32(1)	37(1)	-15(1)	-9(1)	-5(1)
C(30)	49(1)	39(1)	39(1)	-11(1)	-6(1)	-7(1)
C(24)	33(1)	32(1)	37(1)	-16(1)	-5(1)	-4(1)
C(2)	42(1)	41(1)	56(1)	-29(1)	-2(1)	-5(1)
C(3)	44(1)	60(1)	63(1)	-40(1)	0(1)	-14(1)
C(4)	33(1)	73(1)	53(1)	-37(1)	-4(1)	-5(1)
C(5)	39(1)	51(1)	45(1)	-21(1)	-4(1)	3(1)
C(10)	41(1)	37(1)	42(1)	-16(1)	-4(1)	0(1)
C(11)	48(1)	31(1)	46(1)	-16(1)	-4(1)	2(1)
C(17)	49(1)	50(1)	40(1)	-23(1)	8(1)	-6(1)
C(16)	39(1)	40(1)	36(1)	-16(1)	2(1)	-6(1)
C(21)	45(1)	73(1)	49(1)	-29(1)	13(1)	-22(1)
C(23)	37(1)	51(1)	52(1)	-30(1)	5(1)	-11(1)

C(29)	37(1)	33(1)	36(1)	-15(1)	-4(1)	-2(1)
C(28)	36(1)	40(1)	39(1)	-19(1)	-1(1)	-3(1)
C(32)	57(1)	42(1)	38(1)	-11(1)	1(1)	5(1)
B(1)	37(1)	26(1)	34(1)	-10(1)	1(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound 3.

	x	y	z	U(eq)
H(22A)	8046	965	-2132	95
H(22B)	6377	787	-1665	95
H(22C)	7604	-252	-1020	95
H(19A)	5453	903	290	47
H(14A)	6747	-860	2354	55
H(13A)	6023	-2571	2272	56
H(12A)	7362	-4442	3101	50
H(31A)	2561	5405	4115	76
H(31B)	2558	6344	2737	76
H(31C)	3594	6486	3594	76
H(26A)	4665	6227	1300	45
H(30A)	6329	6025	-181	65
H(30B)	6651	4666	-97	65
H(30C)	7821	5255	276	65
H(2A)	9354	4236	2421	52
H(3A)	11610	3992	3113	60
H(4A)	12826	2064	3933	59
H(5A)	11833	393	3987	54
H(10A)	10185	-2896	4112	48
H(11A)	9446	-4592	4006	51
H(17A)	9478	1729	-1165	55
H(21A)	10707	2946	-729	81
H(21B)	10805	2322	694	81
H(21C)	9943	3630	95	81
H(23A)	4343	1279	1849	66

H(23B)	4739	2466	1956	66
H(23C)	5400	1152	2820	66
H(28A)	4414	3724	4714	45
H(32A)	5689	1832	5273	74
H(32B)	7344	2107	4852	74
H(32C)	6569	1410	4276	74

Diagrams showing the structure of **3** with labelling schemes and 50% thermal ellipsoids (bottom), and the intermolecular H-π interactions in the dimer (top).