Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Impact of Constitutional Isomerism on Phosphorescence and Anion-Sensing Properties of Donor-Acceptor Organoboron Pt(II) Complexes

Mei-Ni Belzile, Xiang Wang, Zachary M. Hudson, and Suning Wang*

Department of Chemistry, Queen's University, Kingston, Ontario, K7L 3N6, Canada

S1. Synthesis of starting materials for NBppy

6-bromo-*N,N*-diphenylpyridin-3-amine (1)

The procedure for the synthesis of 6-bromo-*N,N*-diphenylpyridin-3-amine was modified from a previous method described.[28] 1.0 g of 2-bromo-5-iodopyridinium (3.5 mmol, 1.0 equiv.) and 0.59 g of diphenylamine (3.5 mmol, 1.0 equiv.) were placed into a round bottom flask. 64.5 mg of tri(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$) (0.07 mmol, 2 mol%), 87.7 mg of 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (±BINAP) (0.14 mmol, 4 mol%) and 0.44 g of sodium tert-butoxide (4.6 mmol, 1.3 equiv.) were weighed under inert conditions and added to the flask. 10 mL of *m*-xylene solvent, dried over molecular sieves and degassed, was added to the reaction mixture. The reaction was refluxed at 140°C under N_2 for 24 hours. After cooling to room temperature, the reaction was filtered to remove solid impurities and some of the solvent was removed *in vacuo*. Dichloromethane and brine solution were added, and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were dried over $MgSO_4$ and the solvent was removed *in vacuo* to yield a brownish oil. This crude product was purified by column chromatography (DCM: hexanes 1:1, then switching to DCM: hexanes 2:1) and obtained as a yellow-white powder. Yield: 30%. ^{1}H NMR (CD_2Cl_2, 298 K, 400 MHz): δ 8.02 (d, 1H, H-3, J = 2.40 Hz), 7.31 (m, 4H, H-4), 7.29 (m, 1H, H-1), 7.22 (dd, 1H, H-2, J = 3.03, 8.72 Hz), 7.11 (m, 2H, H-6), 7.10 (m, 4H, H-5). HRMS Calcd. for $C_{17}H_{13}BrN_2$ [M^+]: 324.0262, found 324.0255.

6-(4-bromophenyl)-*N,N*-diphenylpyridin-3-amine (2)

The synthesis of 6-(4-bromophenyl)-*N,N*-diphenylpyridin-3-amine was modified from a previous procedure.[29] 0.5 g of 6-bromo-*N,N*-diphenylpyridin-3-amine (**1**) (1.5 mmol, 1.0 equiv.), 0.34 g (1.7 mmol, 1.1 equiv.) of 4-bromophenyl boronic acid, 89.2 mg of tetrakis(triphenylphosphine)-palladium(0) ($Pd(PPh_3)_4$) (0.08 mmol, 5 mol%) and 0.39 g of NaOH (9.6 mmol, 6.25 equiv.) were placed into an evacuated round bottom and placed under vacuum. 15 mL of a 1:1 THF and water degassed solvent mixture was added to the solid reagents and the reaction was allowed to reflux at 55°C under N_2 atmosphere for 24 hours. THF was removed from the reaction mixture *in vacuo*. Dichloromethane and brine solution were added, and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic phases were dried over $MgSO_4$ and the solvent was removed *in vacuo* to yield a yellow oil. This crude product was purified by column chromatography (pure DCM). Yield: 67%. ^{1}H NMR (CD_2Cl_2, 298 K, 400 MHz): δ 8.37 (d, 1H, H-5, J = 2.40 Hz), 7.87 (d, 2H, H-2, J = 8.59 Hz), 7.62 (d, 1H, H-3, J = 8.59 Hz), 7.58 (d, 2H, H-1, J = 8.59 Hz), 7.41 (dd, 1H, H-4, J = 2.78, 8.72 Hz), 7.32 (t, 4H, H-7, J = 7.58 Hz), 7.14 (m, 4H, H-6), 7.10 (m, 2H, H-8). HRMS Calcd. for $C_{23}H_{17}BrN_2$ [M^+]: 402.0558, found 402.0562.

S2. ^{1}H NMR spectra for intermediates, NBppy and Pt-NBppy.

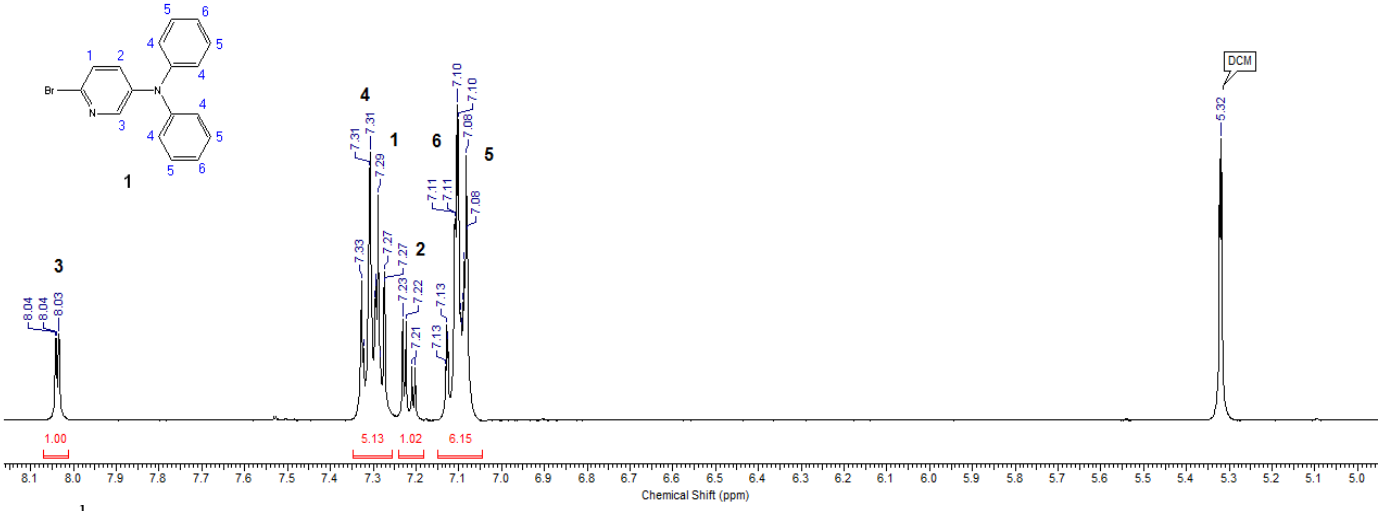


Fig. 1 ^{1}H NMR spectrum for **1** in CD_2Cl_2 at 298K

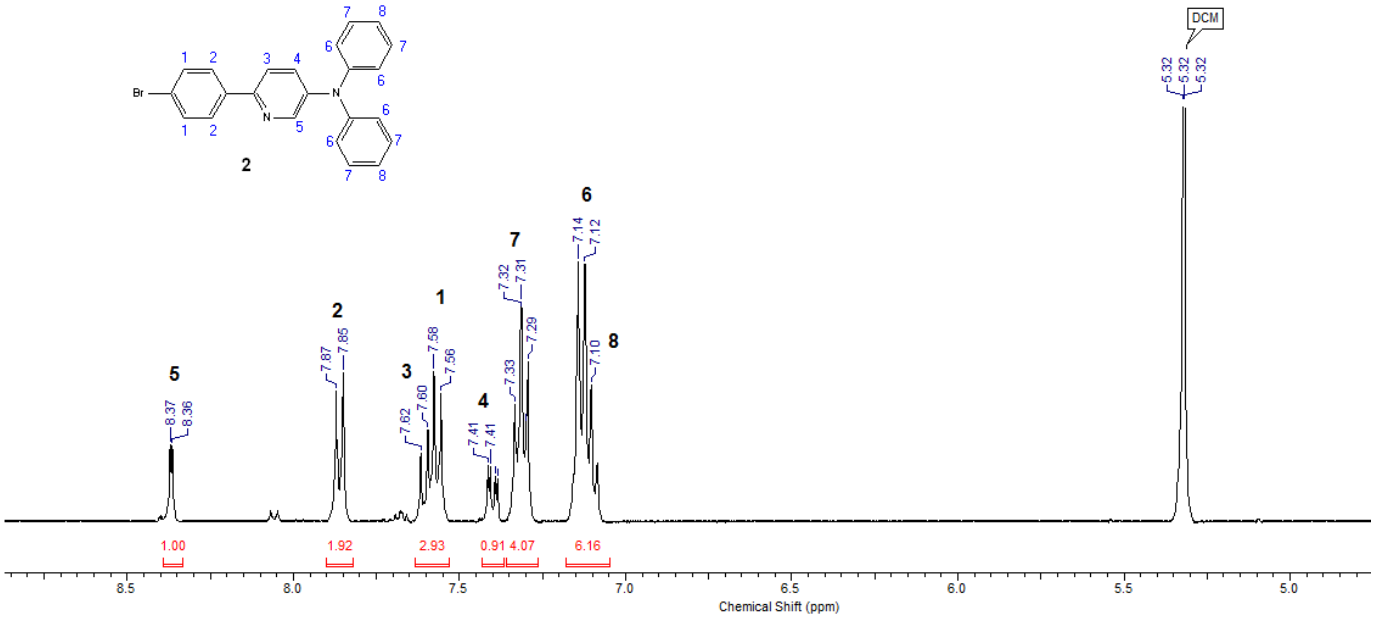


Fig. 2 ^{1}H NMR spectrum for **2** in CD_2Cl_2 at 298K

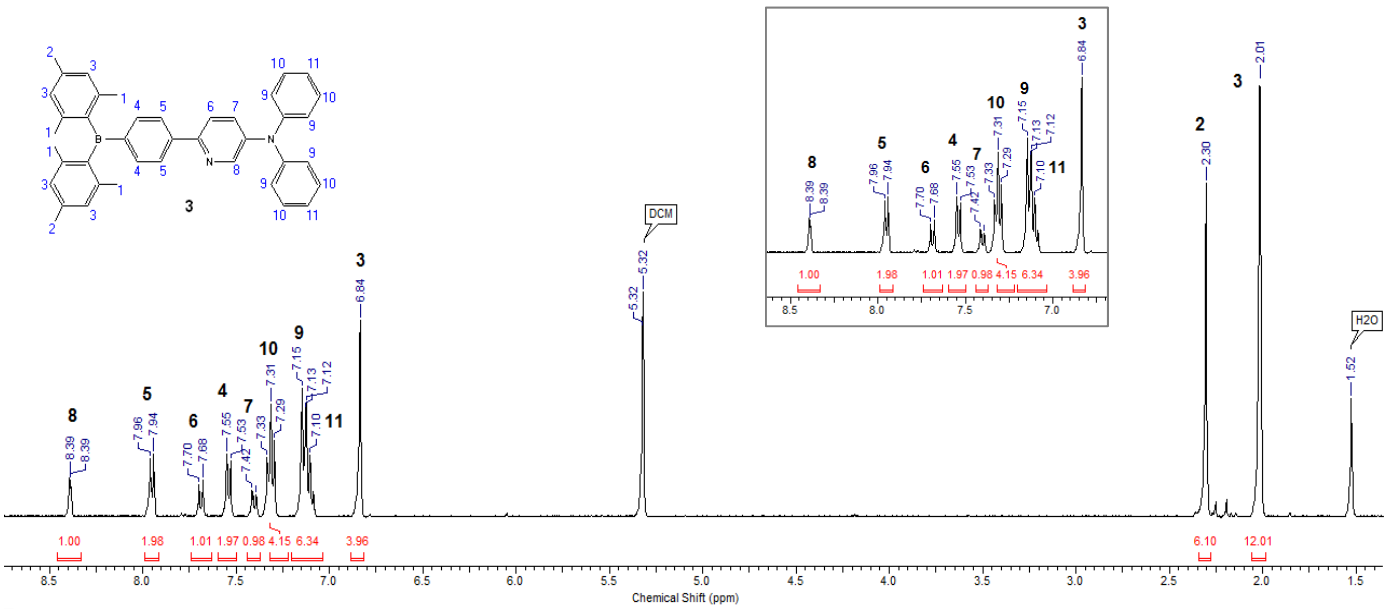


Fig. 3 ^{1}H NMR spectrum for **3** (**NBppy**) in CD_2Cl_2 at 298K (inset shows aromatic region)

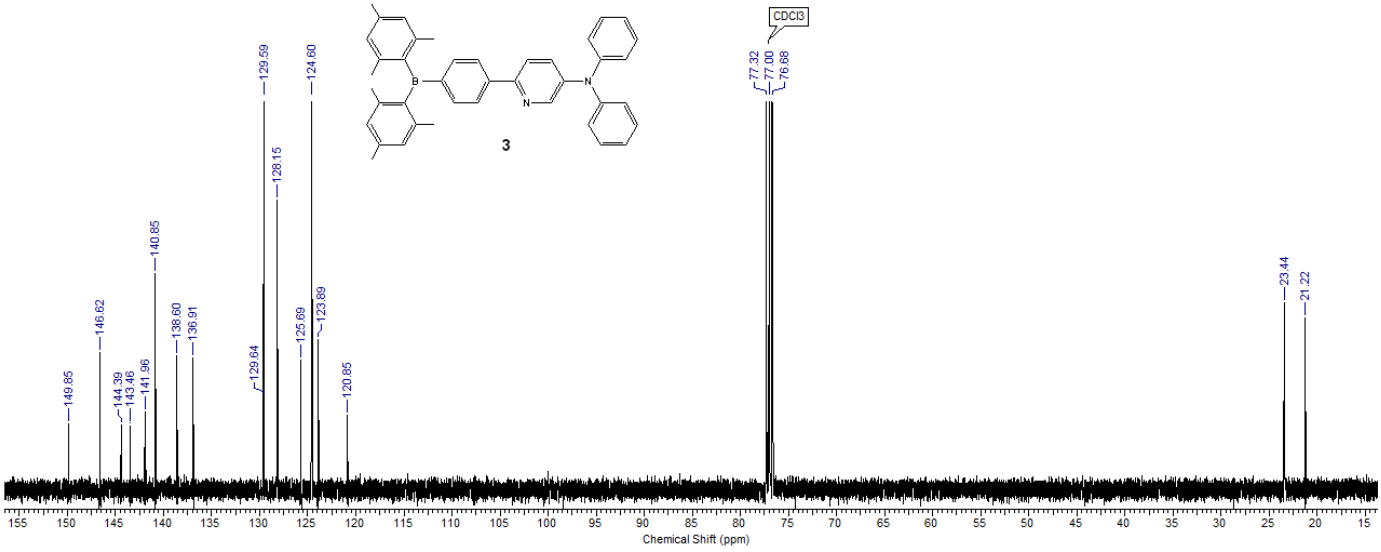


Fig. 4 ^{13}C NMR spectrum for **3** (**NBppy**) in $CDCl_3$ at 298K

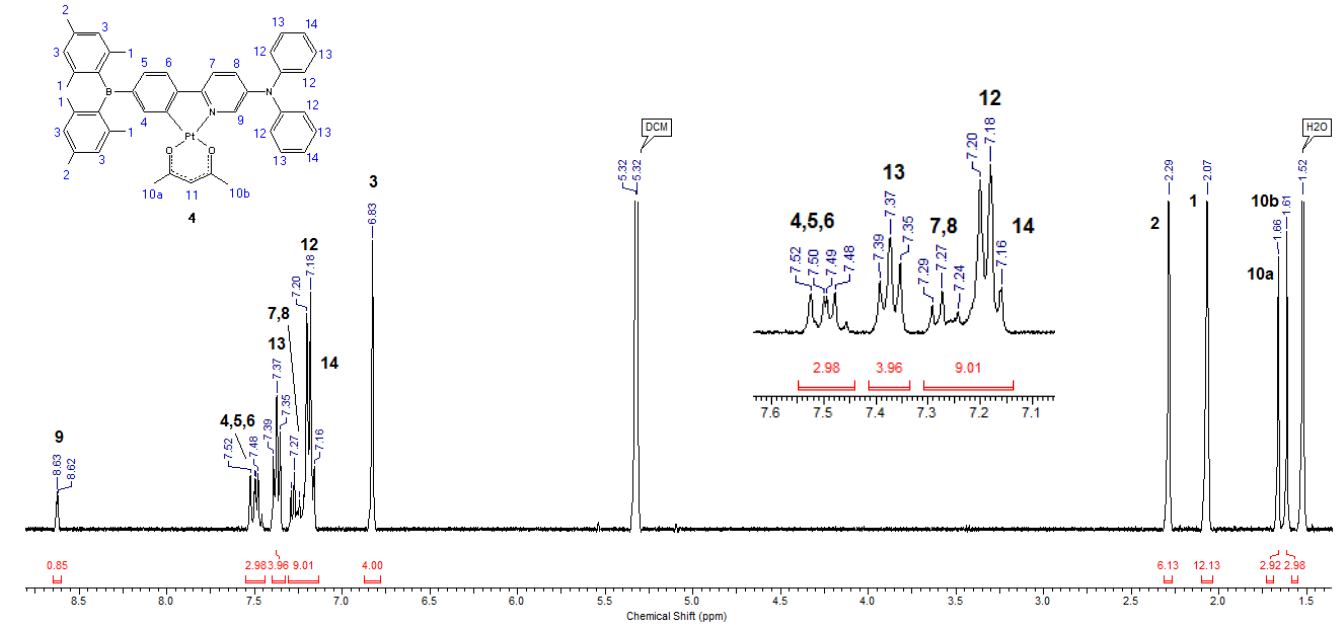


Fig. 5 ^{1}H NMR spectrum for **4** (**Pt-NBppy**) in CD_2Cl_2 at 298K

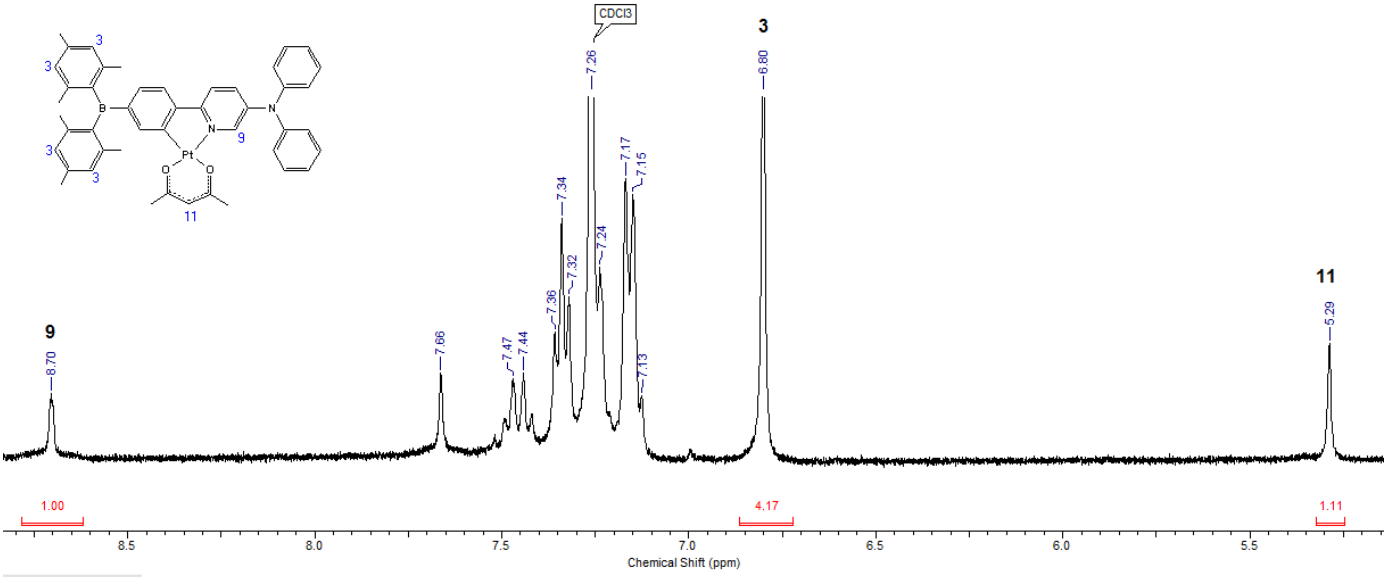


Fig. 6 Aromatic and olefin region of ^{1}H NMR spectrum for **4** (**Pt-NBppy**) in $CDCl_3$ at 298K (shows appearance of H-11)

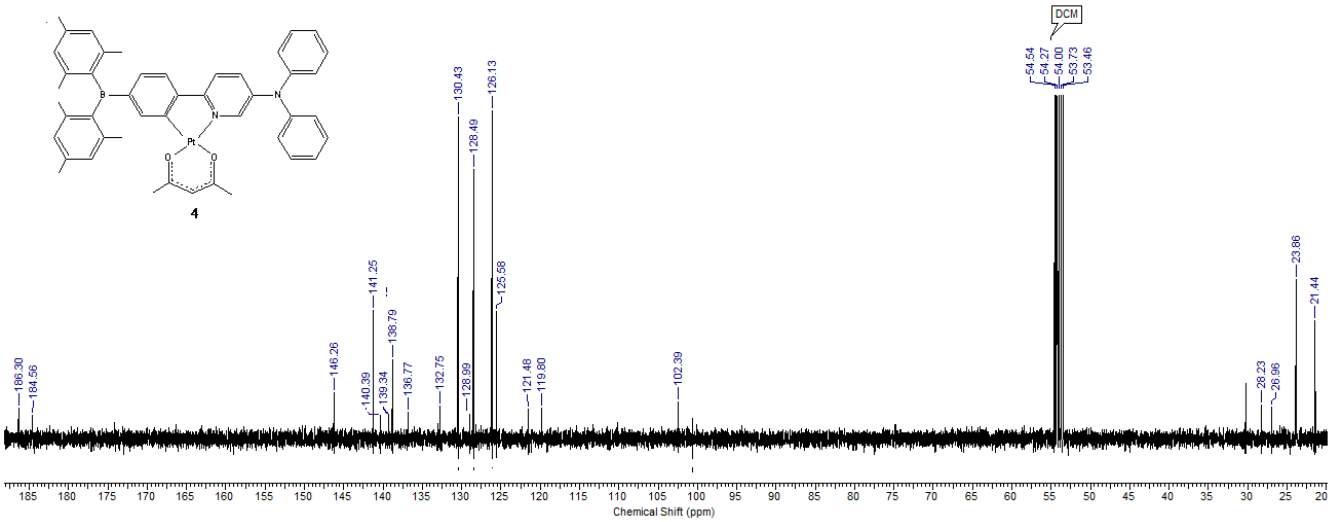


Fig. 7 ^{13}C NMR spectrum for **4** (**Pt-NBppy**) in CD_2Cl_2 at 298K

S3. Absorption and luminescence properties of ligands in solution

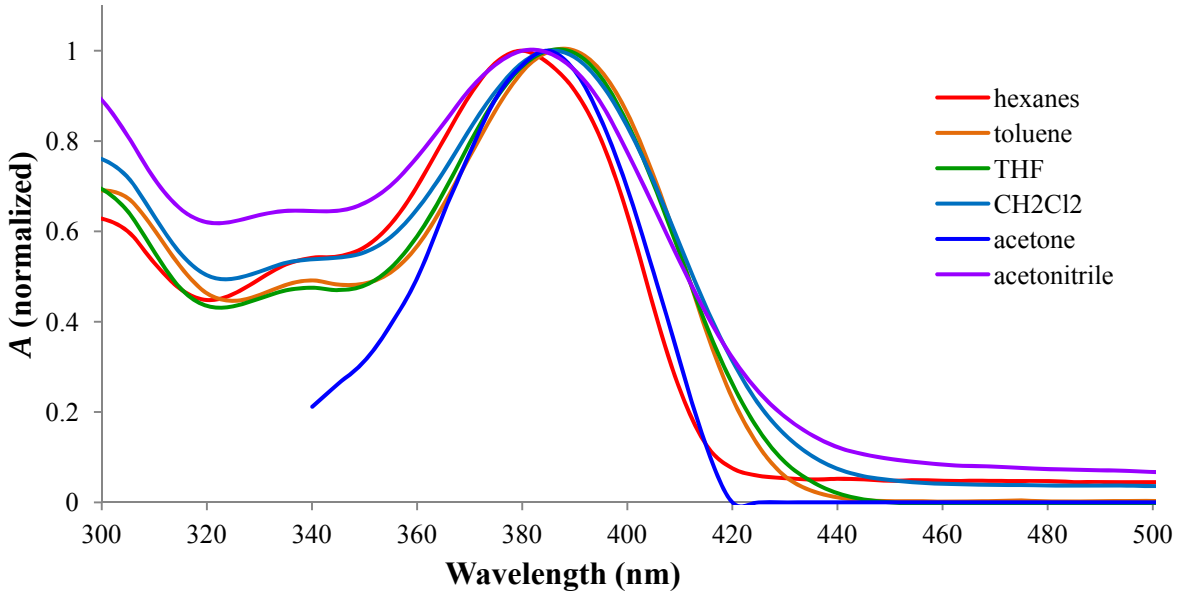


Fig. 10 Normalized absorption spectra for **NBppy** (1×10^{-5} M) in various solvents.

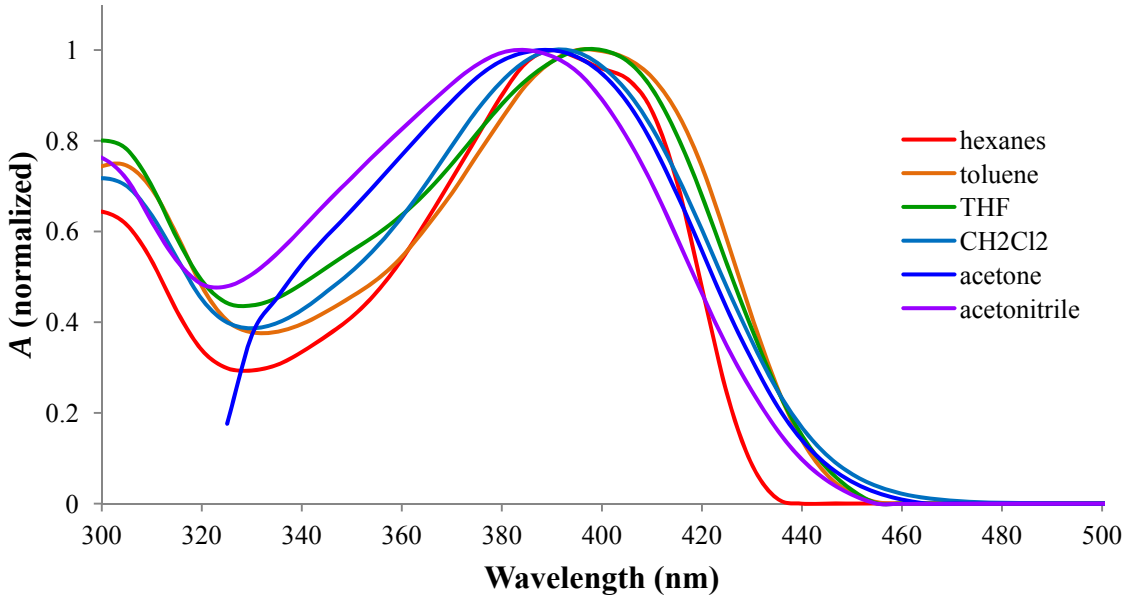


Fig. 12 Normalized absorption spectra for **BNppy** (1×10^{-5} M) in various solvents.

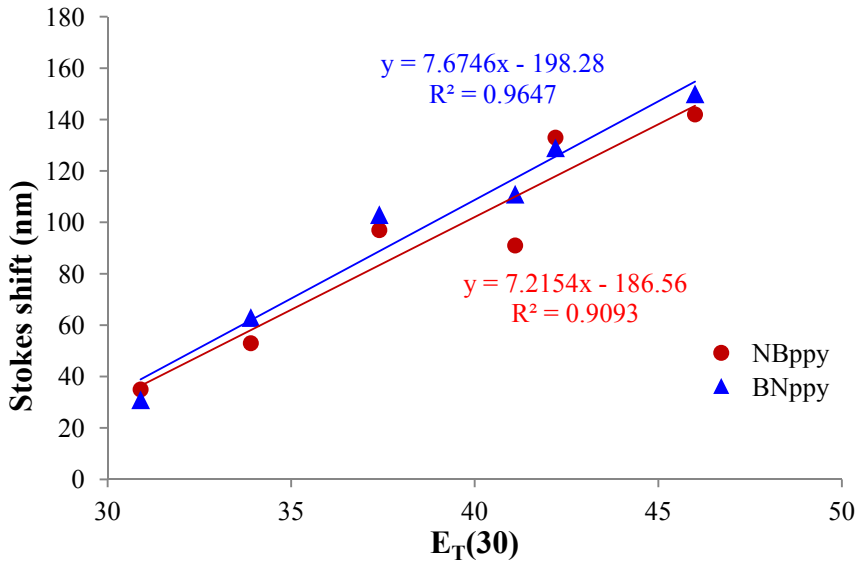


Fig. 13a Plot of Stokes shift versus $E_T(30)$ scale of polarity for **NBppy** and **BNppy** (where Stokes shift is the difference between maximum of excitation and emission spectra).

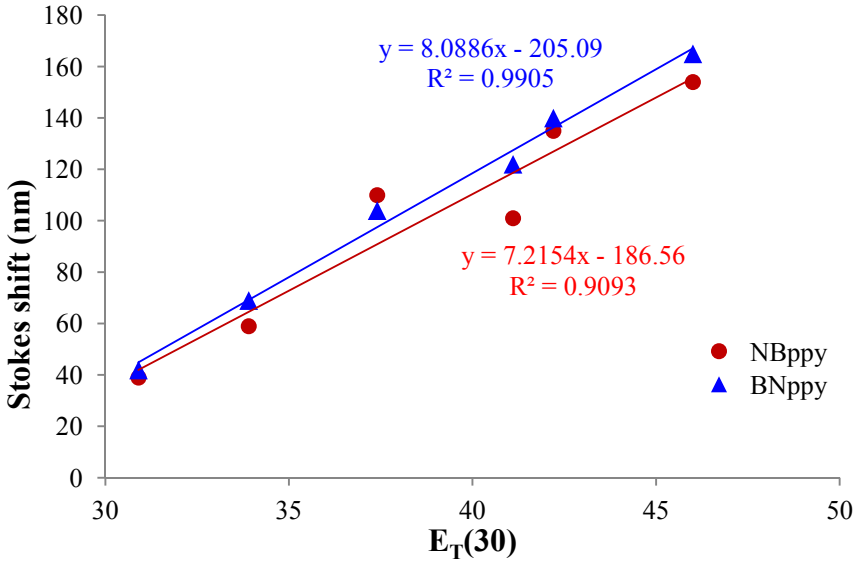
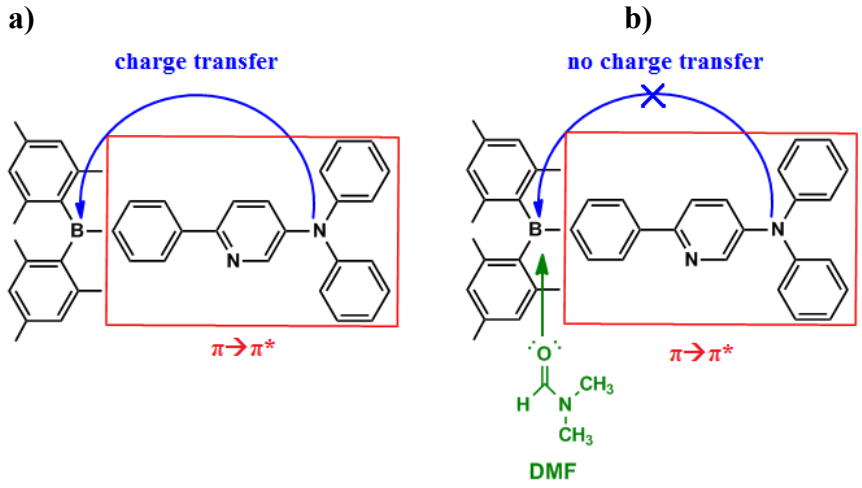


Fig. 13b Plot of Stokes shift versus $E_T(30)$ scale of polarity for **NBppy** and **BNppy** (where Stokes shift is the difference between maximum of absorption and emission spectra).

S4. Fluorescence of NBppy in DMF

NBppy exhibits dual emission properties, where both intramolecular charge transfer (CT) and ligand centered (LC) π→π* transitions are involved (Scheme 1). When in excess (i.e. acting as the solvent), DMF may bind to the boron center, thus quenching the CT emission, such that only emission from the π→π* transitions are observed.



Scheme 1. Diagram illustrating **a)** dual emission present in **NBppy b)** DMF binding to the boron center quenching CT such that only π→π* is observed.

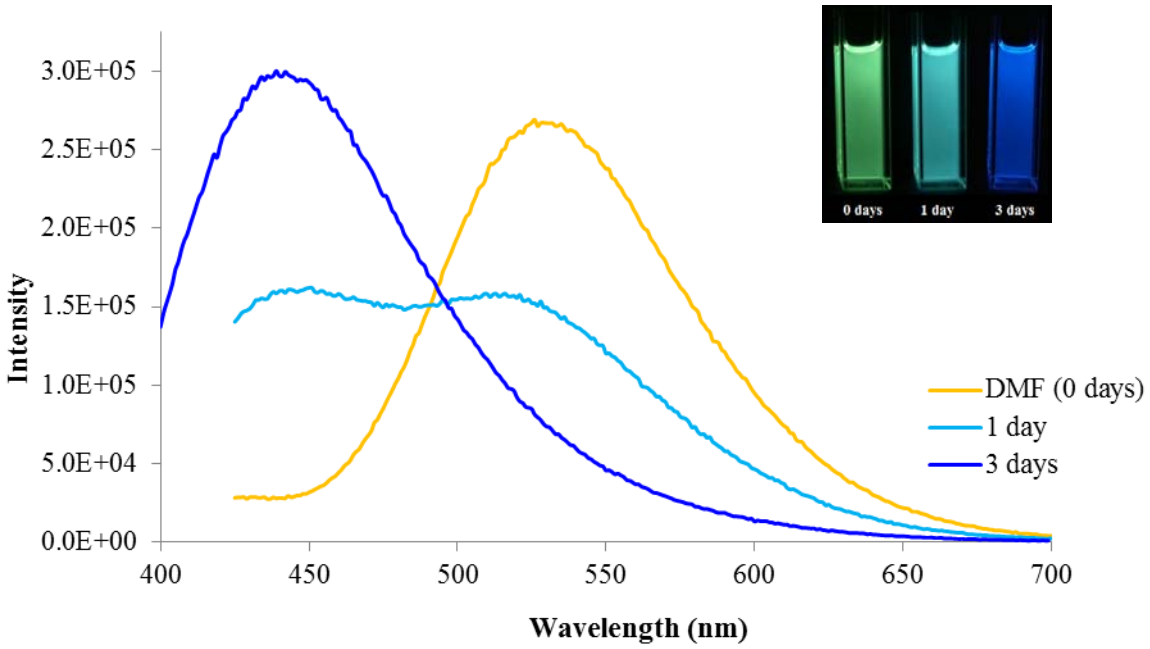


Fig. 14a. Emission spectra showing changes over time of **NBppy** in dry DMF solution. Inset: Photographs of **NBppy** solution under UV irradiation over time.

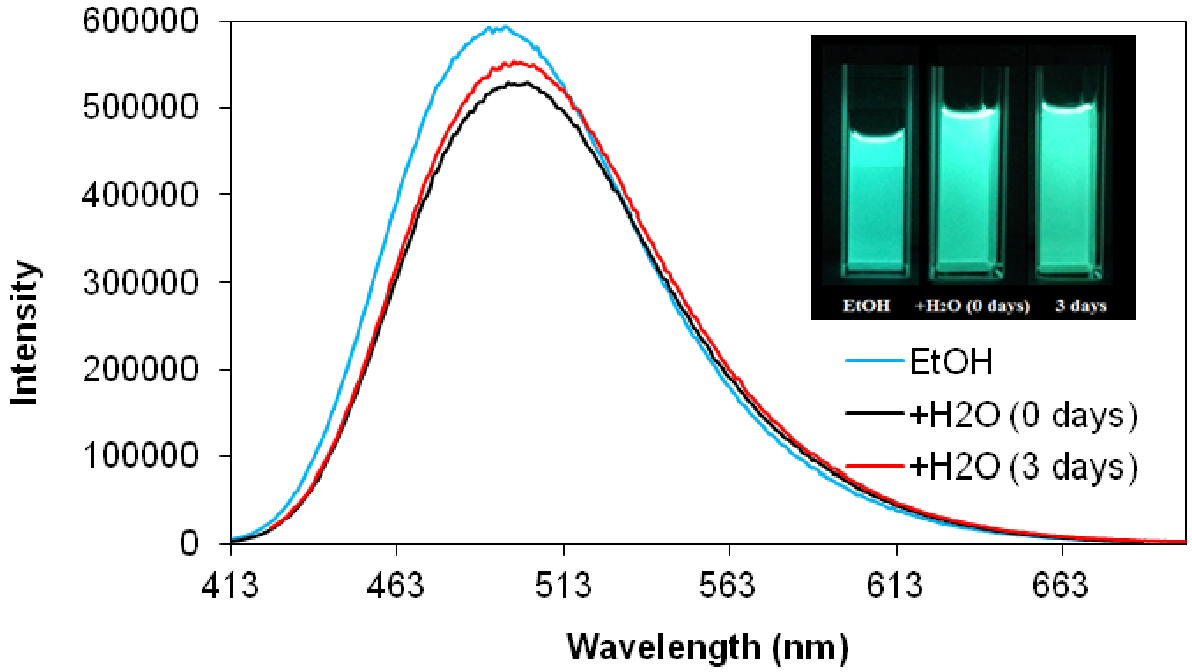


Fig. 14b. Emission spectra showing the effect of adding H_2O to **NBppy** in EtOH. Inset: Photographs of **NBppy** solution under UV irradiation over time.

S5. Absorption and luminescence properties of complexes in solution

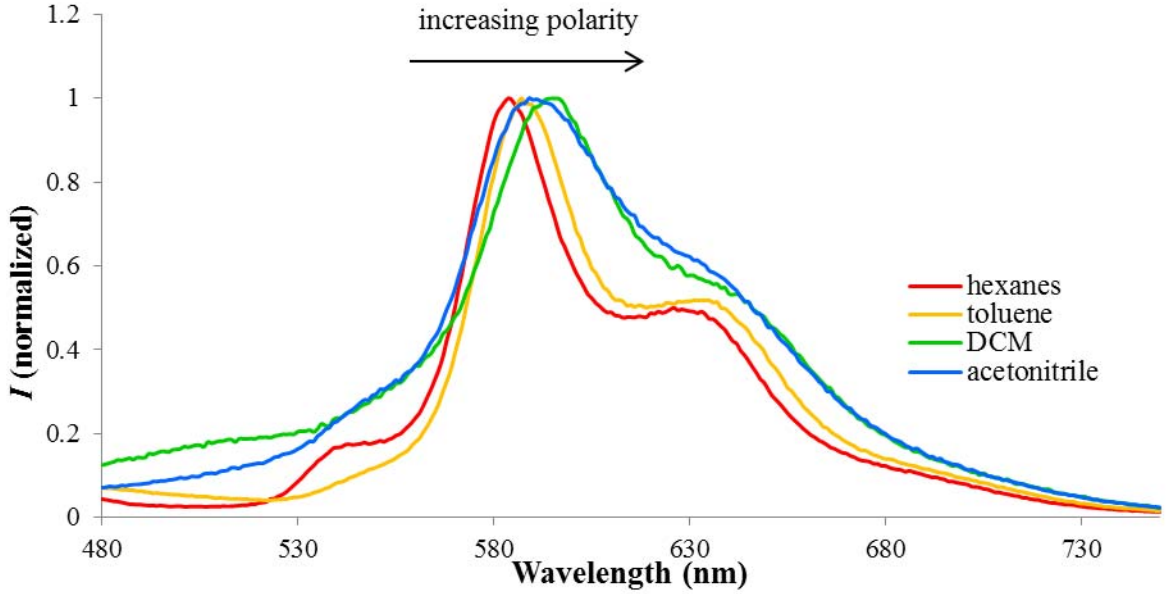


Fig. 16 Normalized emission spectra for **Pt-NBppy** in various solvents. Inset: Photographs of **Pt-NBppy** solutions under irradiation with UV light

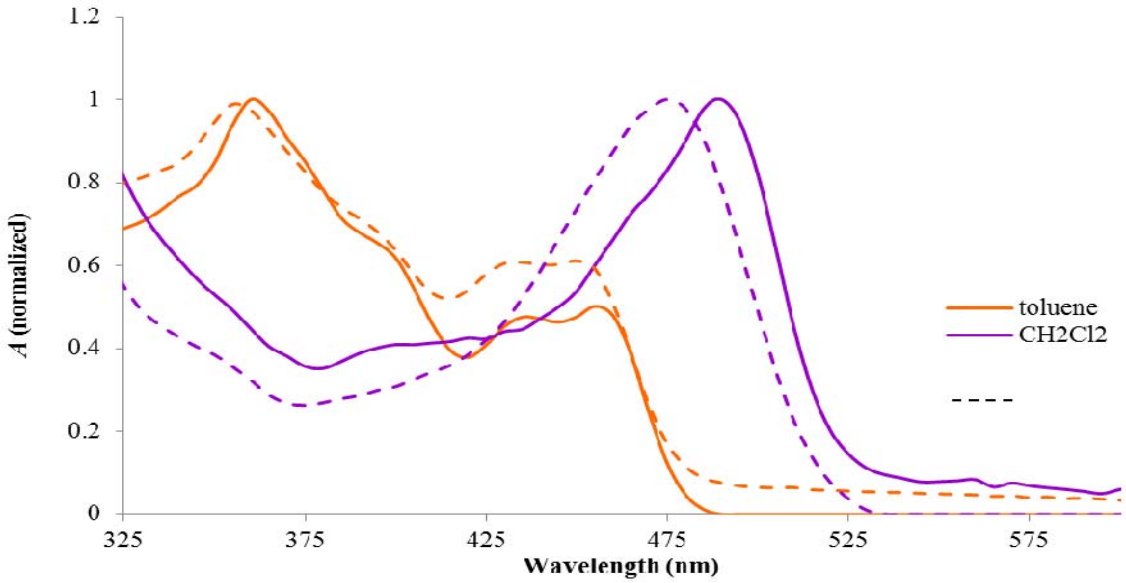


Fig. 17 Absorption spectra of **Pt-NBppy (**orange**)** and **Pt-BNppy** (purple) in toluene (solid line) and CH_2Cl_2 (dashed line).

S6. Fluoride titrations

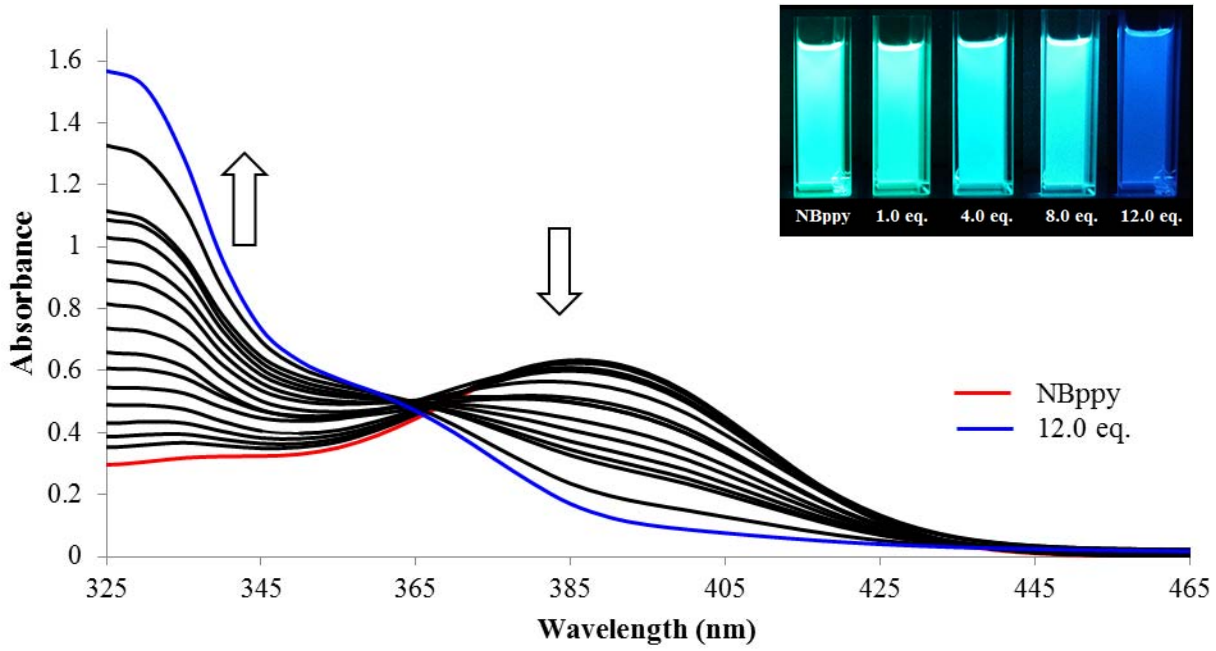


Fig. 18 UV-vis spectral changes for **NBppy** (2×10^{-5} M) with the addition of NBu_4F in CH_2Cl_2. Inset: Photographs of **NBppy** solution throughout F^- titration under UV irradiation.

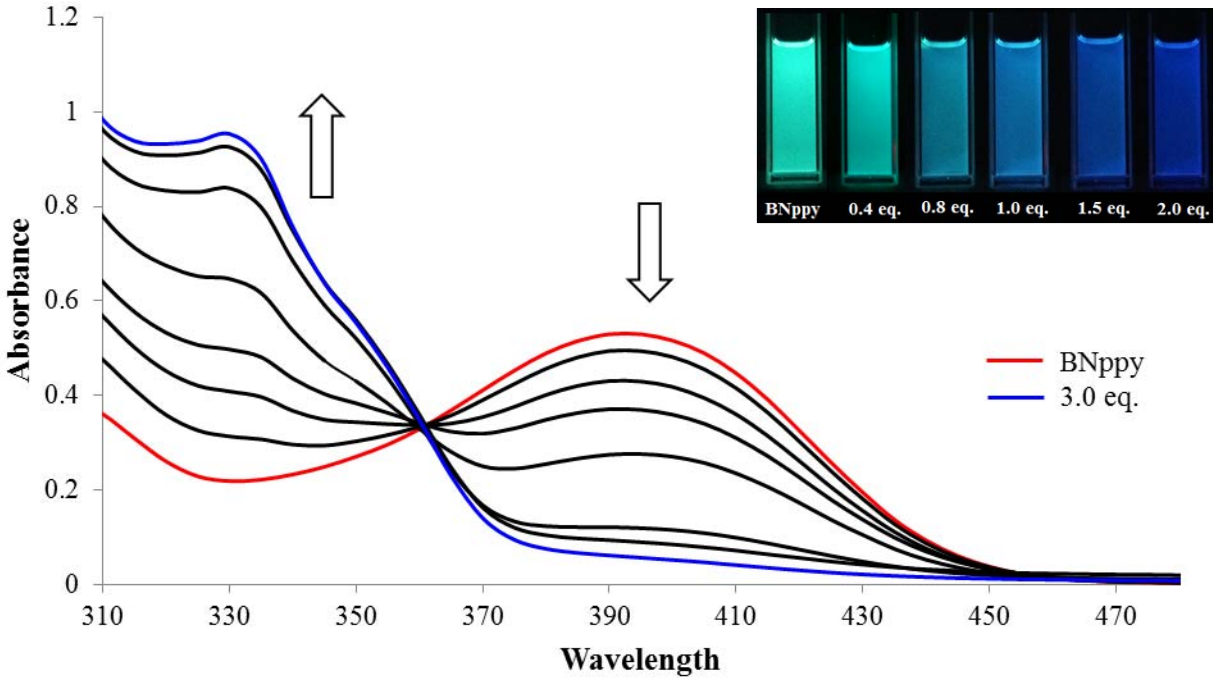


Fig. 19 UV-vis spectral changes for **BNppy** (2×10^{-5} M) with the addition of NBu_4F in CH_2Cl_2. Inset: Photographs of **BNppy** solution throughout F^- titration under UV irradiation.

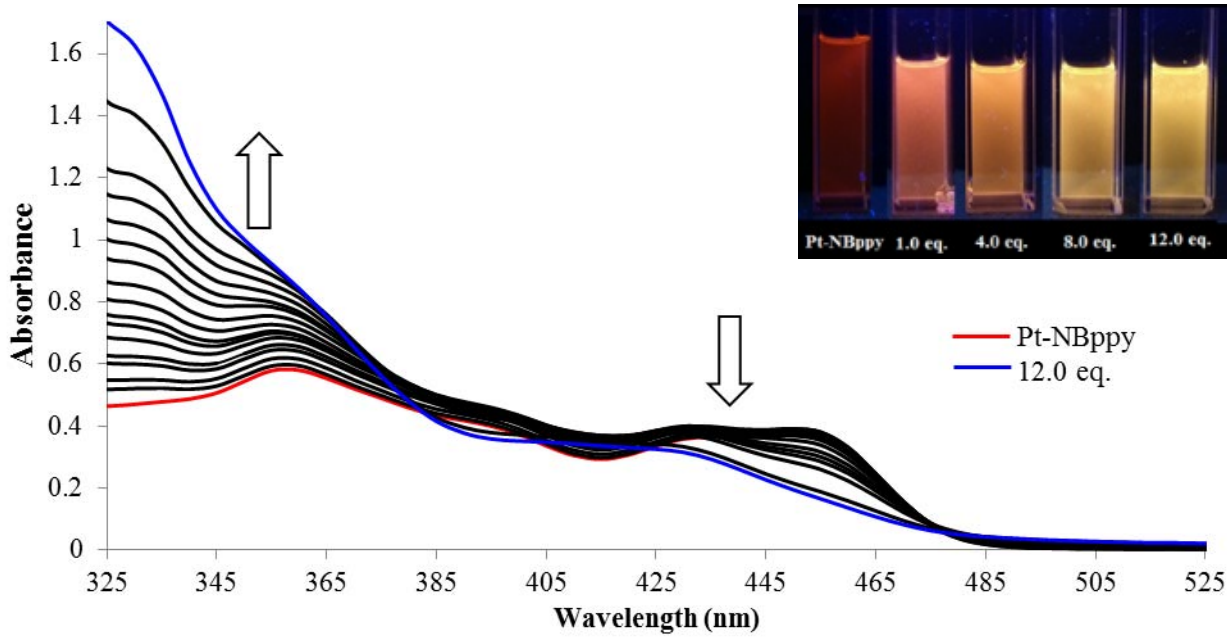


Fig. 20 UV-vis spectral changes for **Pt-NBppy** (2×10^{-5} M) with the addition of NBu_4F in CH_2Cl_2. Inset: Photographs of **Pt-NBppy** solution throughout F^- titration under UV irradiation.

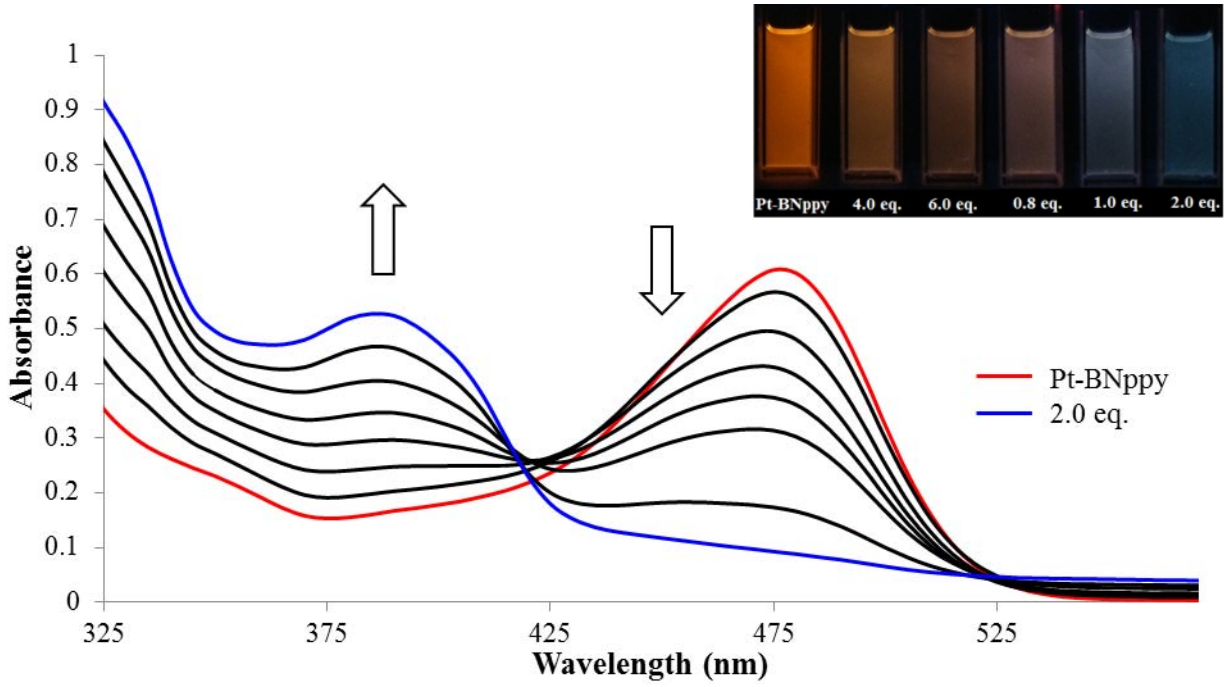


Fig. 21 UV-vis spectral changes for **Pt-BNppy** (2×10^{-5} M) with the addition of NBu_4F in CH_2Cl_2. Inset: Photographs of **Pt-BNppy** solution throughout F^- titration under UV irradiation.

Fluoride titration and Binding constant analysis

A 2×10^{-5} M solution of the free ligand or Pt(II) complex, and NBu_4F solution were prepared in distilled and degassed dichloromethane. Subsequent additions of NBu_4F solution were added to the solution. For the titrations with the Pt(II) complexes, the solutions were degassed under N_2 after each F^- addition. Titrations were monitored by UV-vis, as well as fluorescence and phosphorescence spectroscopy, for the free ligand and platinum complexes, respectively. The binding constants were determined using a least squares fitting method based on a 1:1 binding isotherm utilized previously by Macartney and coworkers[1] in which the binding constant (*K*) and the limiting change in the absorbance intensity ($\Delta A_{limiting}$) are taken as floating parameters. A plot of the predicted change in absorbance versus the corrected fluoride ion concentration was compared with a plot of the observed change in absorbance versus the fluoride ion concentration. The values of $\Delta A_{predicted}$ were calculated based on the 1:1 binding isotherm expressed by **Equations 1-3**. *H* represents the host, which is the cyclometalating ligand or Pt(II) complex, whereas *G* represents the guest molecule, which in this case is the fluoride ion.

$$[H \cdot G] = \frac{b - (b^2 - 4[G]_{total}[H]_{total})^{\frac{1}{2}}}{2} \quad (\mathbf{1})$$

$$\text{where } b = [G]_{total} + [H]_{total} + K^{-1} \quad (\mathbf{2})$$

$$\Delta A_{total} = \Delta A_{limiting}\left(\frac{[H \cdot G]}{[G]_{total}}\right) \quad (\mathbf{3})$$

[1] (a) R. S. Wylie and D. H. Macartney, *Inorg. Chem.*, 1993, **32,** 1830; (b) Y. Li, Y. Kang, J.-S. Lu, I. Wyman, S.-B. Ko and S. Wang. *Organometallics*, 2014, **33**, 964.

Summary of the binding constant of various compounds with fluoride

Compound	Binding constant (M^{-1})
NBppy	$(4.3 \pm 0.4) \times 10^3$
BNppy	$(5.1 \pm 0.5) \times 10^4$
Pt-NBppy	$(1.6 \pm 0.2) \times 10^4$
Pt-BNppy	$(6.5 \pm 0.7) \times 10^4$

Fitting curve for determination of fluoride binding constant

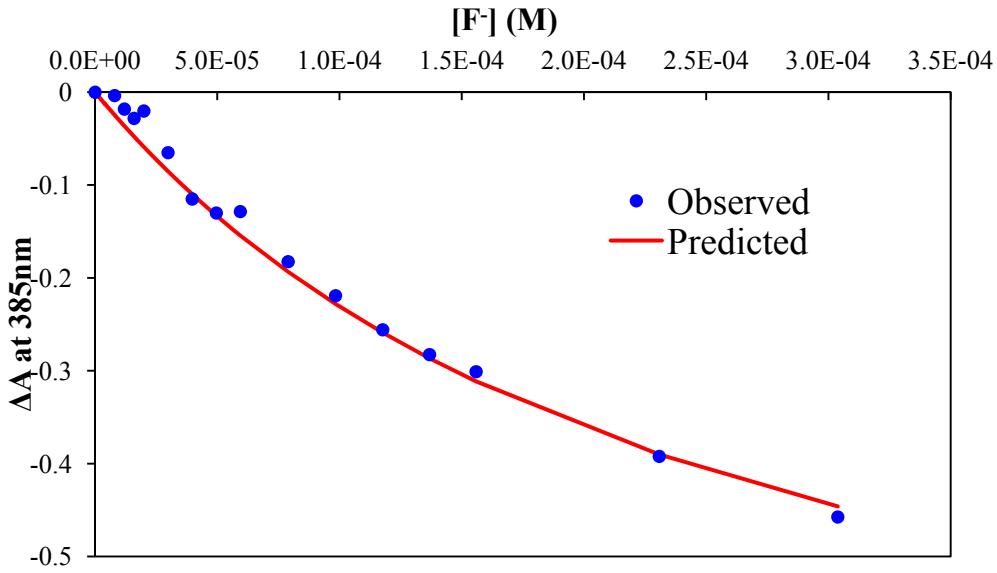


Fig. 22 Plot of the change in absorbance observed at 385 nm exhibited by **NBppy** as a function of the fluoride concentration.

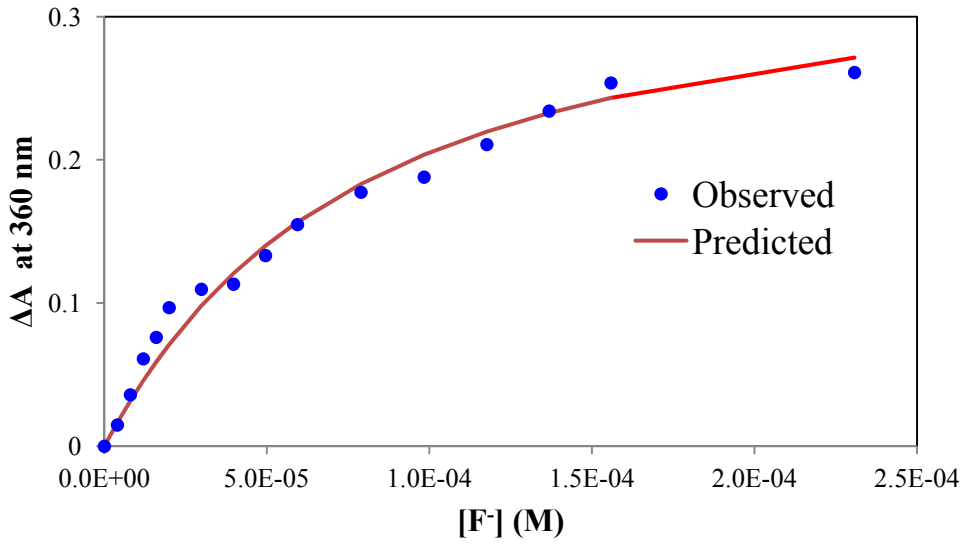


Fig. 23 Plot of the change in absorbance observed at 360 nm exhibited by **Pt-NBppy** as a function of the fluoride concentration.

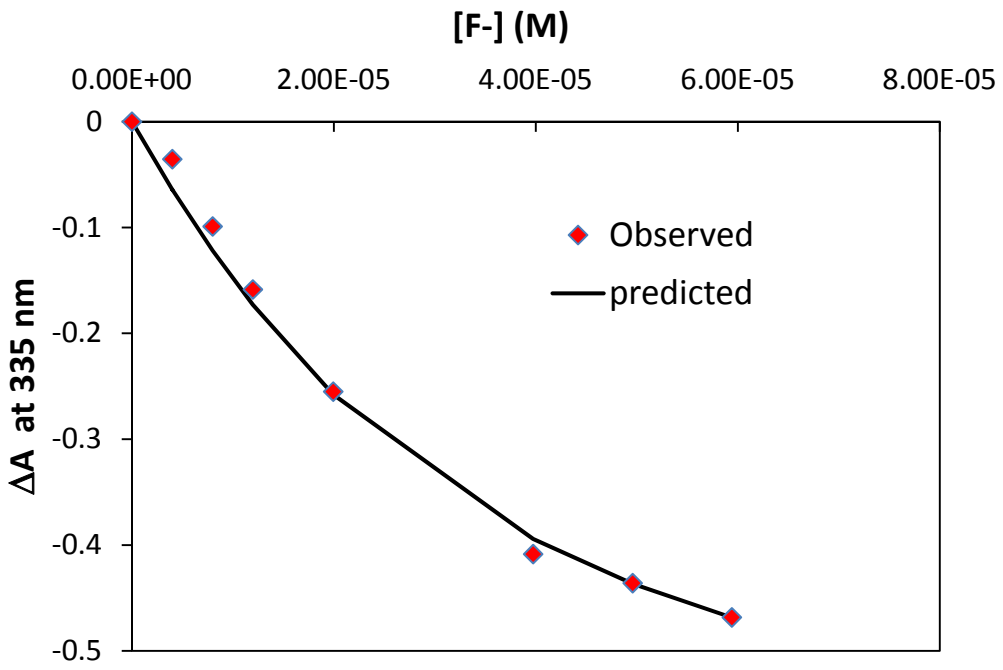


Fig. 24 Plot of the change in absorbance observed at 335 nm exhibited by **BNppy** as a function of the fluoride concentration.

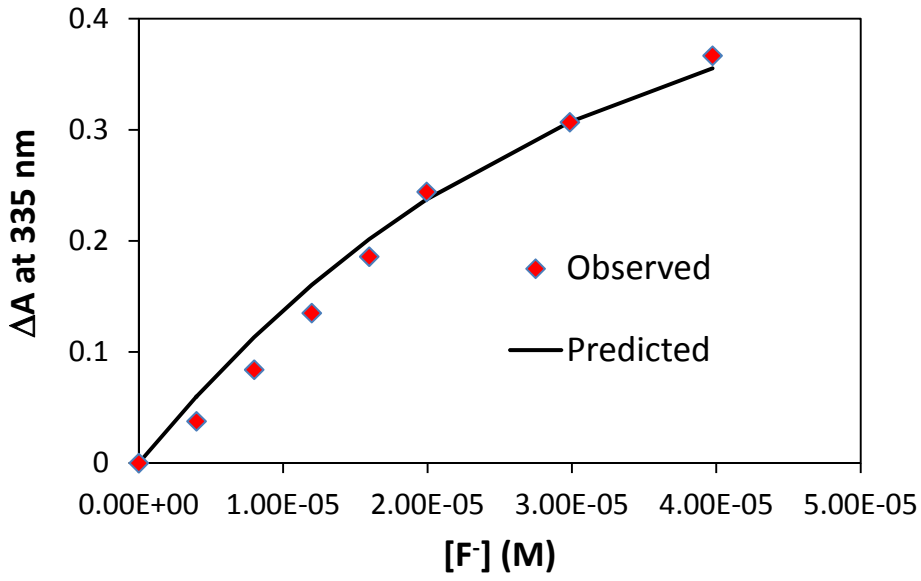


Fig. 25 Plot of the change in absorbance observed at 335 nm exhibited by **Pt-BNppy** as a function of the fluoride concentration.

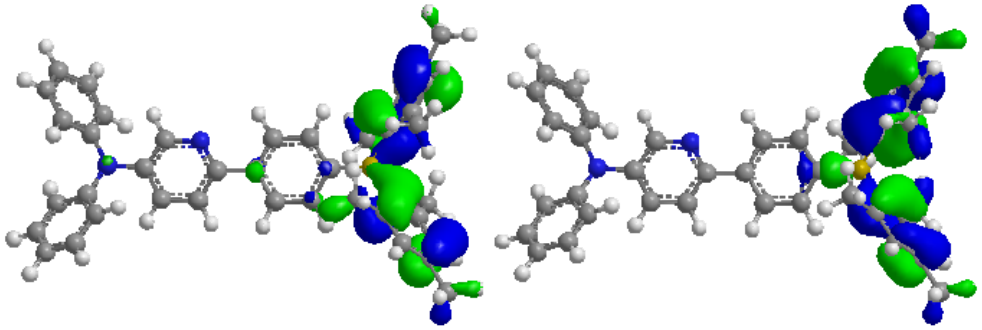
S7. TD-DFT cpmputational data

Table 3. Calculated HOMO and LUMO Energy and Gap of Ligands and Complexes

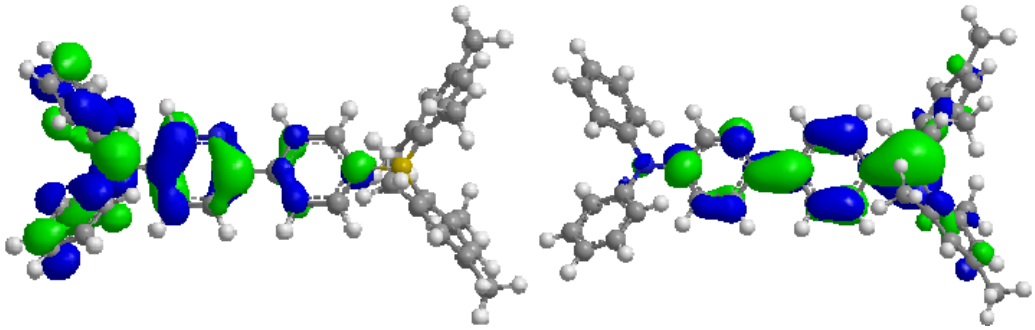
Ligands and Complexes	**Calculated energy (eV)**		
	HOMO	*LUMO*	*Energy gap*
NBppy (3)	-5.12	-1.71	3.41
BNppy	-4.98	-1.85	3.13
Pt-NBppy (4)	-5.14	-1.82	3.32
Pt-BNppy	-4.8	-2.07	2.73

TD-DFT Calculation Results for NBppy

Excited State	Oscillator strength	Transition Energy	Transition configuration
S_1	0.7629	410.88 nm (3.02 eV)	H→L 91%
S_2	0.0681	357.08 nm (3.47 eV)	H-1→L 94%
S_3	0.0267	344.26 nm (3.60 eV)	H-2→L 93%



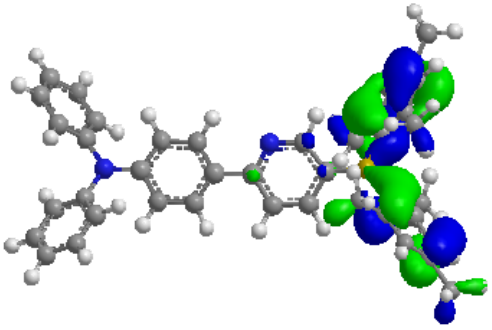
HOMO-2 HOMO-1



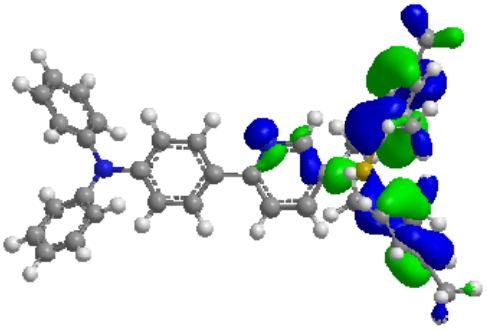
HOMO 5.44 eV LUMO

TD-DFT Calculation Results for BNppy

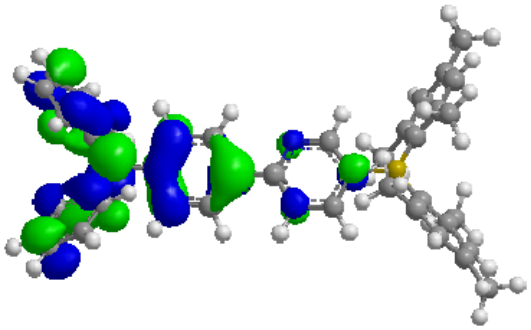
Excited State	Oscillator strength	Transition Energy	Transition configuration
S_1	0.7302	442.16 nm (2.80 eV)	H→L 92%
S_2	0.0564	366.73 nm (3.38 eV)	H-1→L 92%
S_3	0.0361	347.03 nm (3.57 eV)	H-2→L 94%



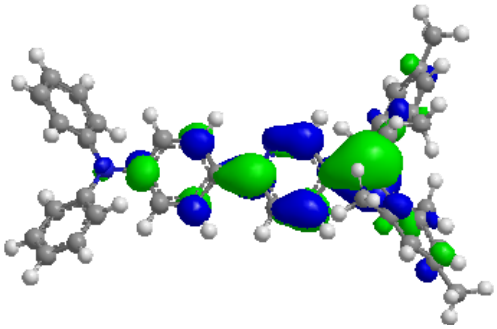
HOMO-2



HOMO-1



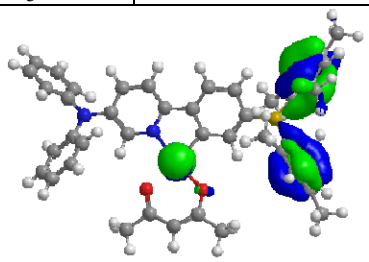
HOMO



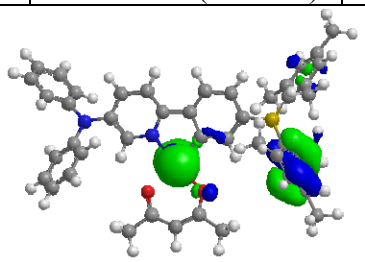
LUMO

TD-DFT Calculation Results for Pt-NBppy

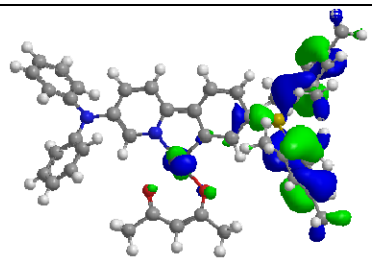
Excited State	Oscillator strength	Transition Energy	Transition configuration
S_1	0.2854	446.20 nm (2.78 eV)	H→L 91%
S_2	0.2700	395.61 nm (3.13 eV)	H-1→L 92%
S_3	0.0191	382.24 nm (3.24 eV)	H-2→L 39% H-5→L 37% H-6→L 13%
T_1	---	560.86 nm (2.21 eV)	H→L 86%
T_2	---	466.41 nm (2.66 eV)	H-1→L 84%
T_3	---	428.53 nm (2.89 eV)	H→L+1 77%



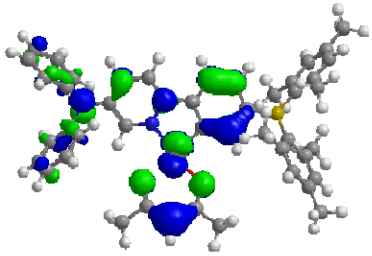
HOMO-6



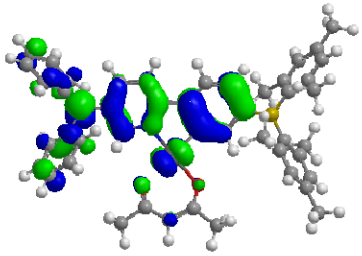
HOMO-5



HOMO-2



HOMO-1



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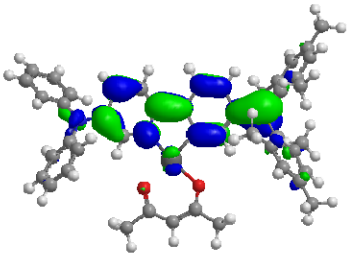
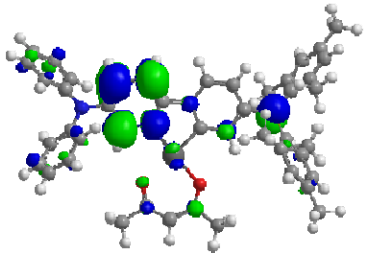


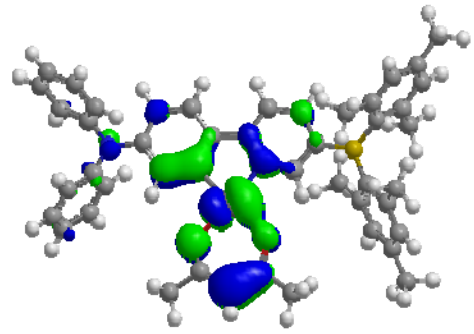
LUMO



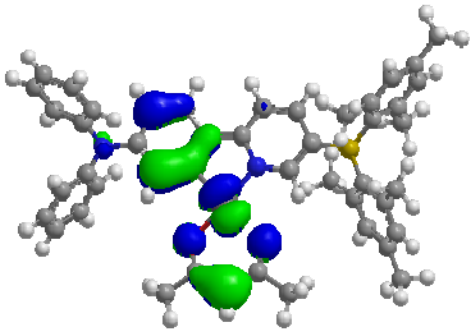
LUMO+1

TD-DFT Calculation Results for Pt-BNppy

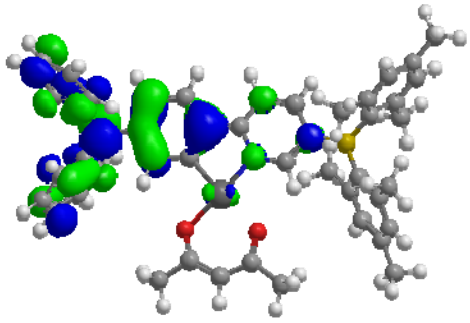
Excited State	Oscillator strength	Transition Energy	Transition configuration
S_1	0.6561	502.28 nm (2.47 eV)	H→L 97%
S_2	0.0212	443.06 nm (2.80 eV)	H-1→L 95%
S_3	0.0087	399.86 nm (3.10 eV)	H-2→L 90%
T_1	---	622.93 nm (1.99 eV)	H→L 88%
T_2	---	474.37 nm (2.61 eV)	H-1→L 91%
T_3	---	432.64 nm (2.87 eV)	H-2→L+4 79%



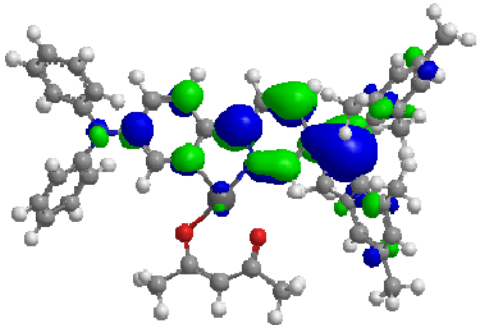
HOMO-2



HOMO-1



HOMO



LUMO

S8. Crystal structural data.

Table 1. Crystal data and structure refinement for NBppy.

Identification code	NBppy	
Empirical formula	C41 H39 B N2	
Formula weight	570.55	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 17.5180(7) Å	α= 90°.
	b = 9.2570(3) Å	β= 109.371(2)°.
	c = 21.2687(7) Å	γ = 90°.
Volume	3253.8(2) $Å^3$	
Z	4	
Density (calculated)	1.165 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	1216	
Crystal size	0.50 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.99 to 26.50°.	
Index ranges	-13<=h<=21, -11<=k<=9, -26<=l<=26	
Reflections collected	19807	
Independent reflections	6700 [R(int) = 0.0825]	
Completeness to theta = 26.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9934 and 0.9675	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6700 / 0 / 404	
Goodness-of-fit on F^2	0.927	
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.1310	
R indices (all data)	R1 = 0.1831, wR2 = 0.1803	
Extinction coefficient	0.0041(7)	
Largest diff. peak and hole	0.236 and -0.238 $e.Å^{-3}$	

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

	x	y	z	U(eq)
B(1)	7154(2)	-475(4)	-457(2)	33(1)
N(1)	10304(2)	3722(3)	852(1)	39(1)
N(2)	11555(2)	6298(3)	2089(1)	38(1)
C(1)	7811(2)	610(3)	-57(2)	33(1)
C(2)	8262(2)	1445(3)	-357(2)	41(1)
C(3)	8869(2)	2375(3)	6(2)	41(1)
C(4)	9024(2)	2556(3)	688(2)	32(1)
C(5)	8571(2)	1779(3)	991(2)	35(1)
C(6)	7988(2)	810(3)	629(2)	36(1)
C(7)	6633(2)	-112(3)	-1195(1)	33(1)
C(8)	6593(2)	-1075(3)	-1724(2)	35(1)
C(9)	6101(2)	-758(3)	-2367(2)	40(1)
C(10)	5622(2)	461(4)	-2524(2)	40(1)
C(11)	5665(2)	1409(3)	-2010(2)	39(1)
C(12)	6166(2)	1175(3)	-1359(2)	36(1)
C(13)	6165(2)	2283(3)	-835(2)	51(1)
C(14)	5059(2)	751(4)	-3223(2)	58(1)
C(15)	7095(2)	-2434(3)	-1596(2)	48(1)
C(16)	7002(2)	-1896(3)	-113(1)	32(1)
C(17)	6222(2)	-2270(3)	-111(1)	32(1)
C(18)	6092(2)	-3547(3)	180(1)	36(1)
C(19)	6709(2)	-4529(3)	467(1)	38(1)
C(20)	7479(2)	-4160(3)	470(2)	42(1)
C(21)	7636(2)	-2876(3)	193(2)	36(1)
C(22)	8501(2)	-2607(4)	227(2)	52(1)
C(23)	5503(2)	-1282(3)	-406(2)	46(1)
C(24)	6548(2)	-5908(3)	776(2)	53(1)
C(25)	9674(2)	3558(3)	1074(2)	31(1)
C(26)	9623(2)	4281(3)	1628(2)	41(1)
C(27)	10243(2)	5204(3)	1967(2)	44(1)
C(28)	10895(2)	5365(3)	1755(2)	36(1)

C(29)	10904(2)	4615(3)	1198(2)	36(1)
C(30)	12291(2)	5635(3)	2493(1)	33(1)
C(31)	12265(2)	4477(3)	2901(1)	35(1)
C(32)	12976(2)	3844(3)	3298(2)	41(1)
C(33)	13712(2)	4358(3)	3300(2)	43(1)
C(34)	13740(2)	5493(4)	2884(2)	47(1)
C(35)	13034(2)	6128(3)	2481(2)	42(1)
C(36)	11422(2)	7800(3)	2074(2)	33(1)
C(37)	10762(2)	8417(3)	1594(2)	41(1)
C(38)	10635(2)	9891(4)	1568(2)	51(1)
C(39)	11167(2)	10787(4)	2023(2)	51(1)
C(40)	11824(2)	10192(4)	2503(2)	49(1)
C(41)	11954(2)	8719(3)	2530(2)	42(1)

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

B(1)-C(1)	1.551(4)	C(7)-C(12)	1.421(4)
B(1)-C(7)	1.568(4)	C(8)-C(9)	1.385(4)
B(1)-C(16)	1.570(5)	C(8)-C(15)	1.507(4)
N(1)-C(25)	1.344(4)	C(9)-C(10)	1.379(4)
N(1)-C(29)	1.347(3)	C(9)-H(9A)	0.9500
N(2)-C(36)	1.409(4)	C(10)-C(11)	1.384(4)
N(2)-C(30)	1.429(3)	C(10)-C(14)	1.511(4)
N(2)-C(28)	1.429(4)	C(11)-C(12)	1.389(4)
C(1)-C(6)	1.399(4)	C(11)-H(11A)	0.9500
C(1)-C(2)	1.402(4)	C(12)-C(13)	1.515(4)
C(2)-C(3)	1.388(4)	C(13)-H(13A)	0.9800
C(2)-H(2A)	0.9500	C(13)-H(13B)	0.9800
C(3)-C(4)	1.394(4)	C(13)-H(13C)	0.9800
C(3)-H(3A)	0.9500	C(14)-H(14A)	0.9800
C(4)-C(5)	1.379(4)	C(14)-H(14B)	0.9800
C(4)-C(25)	1.488(4)	C(14)-H(14C)	0.9800
C(5)-C(6)	1.386(4)	C(15)-H(15A)	0.9800
C(5)-H(5A)	0.9500	C(15)-H(15B)	0.9800
C(6)-H(6A)	0.9500	C(15)-H(15C)	0.9800
C(7)-C(8)	1.419(4)	C(16)-C(17)	1.410(4)

C(16)-C(21)	1.414(4)	C(35)-H(35A)	0.9500
C(17)-C(18)	1.389(4)	C(36)-C(37)	1.387(4)
C(17)-C(23)	1.514(4)	C(36)-C(41)	1.391(4)
C(18)-C(19)	1.389(4)	C(37)-C(38)	1.381(4)
C(18)-H(18A)	0.9500	C(37)-H(37A)	0.9500
C(19)-C(20)	1.390(4)	C(38)-C(39)	1.377(4)
C(19)-C(24)	1.504(4)	C(38)-H(38A)	0.9500
C(20)-C(21)	1.394(4)	C(39)-C(40)	1.375(4)
C(20)-H(20A)	0.9500	C(39)-H(39A)	0.9500
C(21)-C(22)	1.515(4)	C(40)-C(41)	1.380(4)
C(22)-H(22A)	0.9800	C(40)-H(40A)	0.9500
C(22)-H(22B)	0.9800	C(41)-H(41A)	0.9500
C(22)-H(22C)	0.9800		
C(23)-H(23A)	0.9800	C(1)-B(1)-C(7)	119.3(3)
C(23)-H(23B)	0.9800	C(1)-B(1)-C(16)	119.7(3)
C(23)-H(23C)	0.9800	C(7)-B(1)-C(16)	120.9(3)
C(24)-H(24A)	0.9800	C(25)-N(1)-C(29)	117.4(3)
C(24)-H(24B)	0.9800	C(36)-N(2)-C(30)	123.2(2)
C(24)-H(24C)	0.9800	C(36)-N(2)-C(28)	119.0(2)
C(25)-C(26)	1.385(4)	C(30)-N(2)-C(28)	117.4(2)
C(26)-C(27)	1.383(4)	C(6)-C(1)-C(2)	116.0(3)
C(26)-H(26A)	0.9500	C(6)-C(1)-B(1)	121.7(3)
C(27)-C(28)	1.368(4)	C(2)-C(1)-B(1)	122.3(3)
C(27)-H(27A)	0.9500	C(3)-C(2)-C(1)	122.2(3)
C(28)-C(29)	1.378(4)	C(3)-C(2)-H(2A)	118.9
C(29)-H(29A)	0.9500	C(1)-C(2)-H(2A)	118.9
C(30)-C(35)	1.387(4)	C(2)-C(3)-C(4)	120.1(3)
C(30)-C(31)	1.389(4)	C(2)-C(3)-H(3A)	119.9
C(31)-C(32)	1.382(4)	C(4)-C(3)-H(3A)	119.9
C(31)-H(31A)	0.9500	C(5)-C(4)-C(3)	118.8(3)
C(32)-C(33)	1.372(4)	C(5)-C(4)-C(25)	121.4(3)
C(32)-H(32A)	0.9500	C(3)-C(4)-C(25)	119.8(3)
C(33)-C(34)	1.385(4)	C(4)-C(5)-C(6)	120.7(3)
C(33)-H(33A)	0.9500	C(4)-C(5)-H(5A)	119.7
C(34)-C(35)	1.381(4)	C(6)-C(5)-H(5A)	119.7
C(34)-H(34A)	0.9500	C(5)-C(6)-C(1)	122.2(3)

C(5)-C(6)-H(6A)	118.9	H(15A)-C(15)-H(15C)	109.5
C(1)-C(6)-H(6A)	118.9	H(15B)-C(15)-H(15C)	109.5
C(8)-C(7)-C(12)	117.3(3)	C(17)-C(16)-C(21)	117.1(3)
C(8)-C(7)-B(1)	121.2(3)	C(17)-C(16)-B(1)	121.4(3)
C(12)-C(7)-B(1)	121.4(3)	C(21)-C(16)-B(1)	121.5(3)
C(9)-C(8)-C(7)	120.1(3)	C(18)-C(17)-C(16)	120.8(3)
C(9)-C(8)-C(15)	119.3(3)	C(18)-C(17)-C(23)	117.5(3)
C(7)-C(8)-C(15)	120.6(3)	C(16)-C(17)-C(23)	121.6(3)
C(10)-C(9)-C(8)	122.8(3)	C(17)-C(18)-C(19)	122.3(3)
C(10)-C(9)-H(9A)	118.6	C(17)-C(18)-H(18A)	118.8
C(8)-C(9)-H(9A)	118.6	C(19)-C(18)-H(18A)	118.8
C(9)-C(10)-C(11)	117.3(3)	C(18)-C(19)-C(20)	117.0(3)
C(9)-C(10)-C(14)	121.9(3)	C(18)-C(19)-C(24)	121.1(3)
C(11)-C(10)-C(14)	120.8(3)	C(20)-C(19)-C(24)	121.9(3)
C(10)-C(11)-C(12)	122.6(3)	C(19)-C(20)-C(21)	122.3(3)
C(10)-C(11)-H(11A)	118.7	C(19)-C(20)-H(20A)	118.9
C(12)-C(11)-H(11A)	118.7	C(21)-C(20)-H(20A)	118.9
C(11)-C(12)-C(7)	119.8(3)	C(20)-C(21)-C(16)	120.5(3)
C(11)-C(12)-C(13)	118.2(3)	C(20)-C(21)-C(22)	117.0(3)
C(7)-C(12)-C(13)	121.9(3)	C(16)-C(21)-C(22)	122.5(3)
C(12)-C(13)-H(13A)	109.5	C(21)-C(22)-H(22A)	109.5
C(12)-C(13)-H(13B)	109.5	C(21)-C(22)-H(22B)	109.5
H(13A)-C(13)-H(13B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(12)-C(13)-H(13C)	109.5	C(21)-C(22)-H(22C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(13B)-C(13)-H(13C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(10)-C(14)-H(14A)	109.5	C(17)-C(23)-H(23A)	109.5
C(10)-C(14)-H(14B)	109.5	C(17)-C(23)-H(23B)	109.5
H(14A)-C(14)-H(14B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(10)-C(14)-H(14C)	109.5	C(17)-C(23)-H(23C)	109.5
H(14A)-C(14)-H(14C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(14B)-C(14)-H(14C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(8)-C(15)-H(15A)	109.5	C(19)-C(24)-H(24A)	109.5
C(8)-C(15)-H(15B)	109.5	C(19)-C(24)-H(24B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(8)-C(15)-H(15C)	109.5	C(19)-C(24)-H(24C)	109.5

H(24A)-C(24)-H(24C)	109.5	C(32)-C(33)-H(33A)	120.2
H(24B)-C(24)-H(24C)	109.5	C(34)-C(33)-H(33A)	120.2
N(1)-C(25)-C(26)	122.4(3)	C(35)-C(34)-C(33)	120.3(3)
N(1)-C(25)-C(4)	116.5(3)	C(35)-C(34)-H(34A)	119.8
C(26)-C(25)-C(4)	121.1(3)	C(33)-C(34)-H(34A)	119.8
C(27)-C(26)-C(25)	118.7(3)	C(34)-C(35)-C(30)	120.1(3)
C(27)-C(26)-H(26A)	120.6	C(34)-C(35)-H(35A)	120.0
C(25)-C(26)-H(26A)	120.6	C(30)-C(35)-H(35A)	120.0
C(28)-C(27)-C(26)	119.5(3)	C(37)-C(36)-C(41)	117.7(3)
C(28)-C(27)-H(27A)	120.3	C(37)-C(36)-N(2)	121.0(3)
C(26)-C(27)-H(27A)	120.3	C(41)-C(36)-N(2)	121.4(3)
C(27)-C(28)-C(29)	118.6(3)	C(38)-C(37)-C(36)	121.3(3)
C(27)-C(28)-N(2)	121.9(3)	C(38)-C(37)-H(37A)	119.3
C(29)-C(28)-N(2)	119.6(3)	C(36)-C(37)-H(37A)	119.3
N(1)-C(29)-C(28)	123.3(3)	C(39)-C(38)-C(37)	120.3(3)
N(1)-C(29)-H(29A)	118.4	C(39)-C(38)-H(38A)	119.8
C(28)-C(29)-H(29A)	118.4	C(37)-C(38)-H(38A)	119.8
C(35)-C(30)-C(31)	119.4(3)	C(40)-C(39)-C(38)	119.0(3)
C(35)-C(30)-N(2)	120.8(3)	C(40)-C(39)-H(39A)	120.5
C(31)-C(30)-N(2)	119.8(3)	C(38)-C(39)-H(39A)	120.5
C(32)-C(31)-C(30)	119.9(3)	C(39)-C(40)-C(41)	120.9(3)
C(32)-C(31)-H(31A)	120.0	C(39)-C(40)-H(40A)	119.6
C(30)-C(31)-H(31A)	120.0	C(41)-C(40)-H(40A)	119.6
C(33)-C(32)-C(31)	120.7(3)	C(40)-C(41)-C(36)	120.8(3)
C(33)-C(32)-H(32A)	119.7	C(40)-C(41)-H(41A)	119.6
C(31)-C(32)-H(32A)	119.7	C(36)-C(41)-H(41A)	119.6
C(32)-C(33)-C(34)	119.6(3)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for NBppy. 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}
B(1)	26(2)	40(2)	36(2)	-8(2)	12(2)	5(2)
N(1)	33(2)	40(2)	45(2)	-1(1)	13(1)	-7(1)
N(2)	29(2)	30(2)	48(2)	-2(1)	1(1)	-2(1)

C(1)	35(2)	36(2)	29(2)	1(2)	10(2)	-3(2)
C(2)	46(2)	51(2)	28(2)	-3(2)	13(2)	-9(2)
C(3)	42(2)	48(2)	37(2)	0(2)	16(2)	-13(2)
C(4)	29(2)	34(2)	33(2)	-2(2)	9(2)	-1(2)
C(5)	34(2)	40(2)	26(2)	-2(2)	5(2)	-5(2)
C(6)	32(2)	43(2)	35(2)	2(2)	14(2)	-9(2)
C(7)	30(2)	35(2)	33(2)	0(2)	10(2)	-3(2)
C(8)	31(2)	37(2)	37(2)	-1(2)	10(2)	-1(2)
C(9)	40(2)	43(2)	33(2)	-7(2)	10(2)	-8(2)
C(10)	37(2)	47(2)	32(2)	5(2)	6(2)	-11(2)
C(11)	33(2)	36(2)	46(2)	5(2)	10(2)	-2(2)
C(12)	31(2)	40(2)	34(2)	2(2)	9(2)	-6(2)
C(13)	55(2)	46(2)	50(2)	-7(2)	13(2)	9(2)
C(14)	63(3)	62(2)	38(2)	6(2)	3(2)	-2(2)
C(15)	52(2)	45(2)	42(2)	-6(2)	11(2)	6(2)
C(16)	27(2)	34(2)	32(2)	-4(2)	6(2)	-2(2)
C(17)	34(2)	33(2)	27(2)	-7(2)	6(2)	-2(2)
C(18)	30(2)	41(2)	38(2)	-5(2)	13(2)	-4(2)
C(19)	41(2)	35(2)	30(2)	0(2)	2(2)	-2(2)
C(20)	38(2)	41(2)	40(2)	3(2)	5(2)	7(2)
C(21)	29(2)	42(2)	34(2)	-4(2)	7(2)	0(2)
C(22)	33(2)	56(2)	63(2)	4(2)	9(2)	5(2)
C(23)	31(2)	41(2)	66(2)	3(2)	18(2)	3(2)
C(24)	58(3)	49(2)	49(2)	9(2)	13(2)	3(2)
C(25)	26(2)	28(2)	37(2)	1(2)	8(2)	0(2)
C(26)	31(2)	49(2)	45(2)	-7(2)	16(2)	-8(2)
C(27)	40(2)	50(2)	43(2)	-11(2)	15(2)	-8(2)
C(28)	29(2)	32(2)	41(2)	-1(2)	5(2)	-4(2)
C(29)	27(2)	36(2)	43(2)	0(2)	8(2)	-2(2)
C(30)	30(2)	29(2)	36(2)	-4(2)	6(2)	0(2)
C(31)	30(2)	41(2)	35(2)	-5(2)	11(2)	-4(2)
C(32)	48(2)	36(2)	35(2)	0(2)	9(2)	0(2)
C(33)	38(2)	41(2)	42(2)	-5(2)	2(2)	1(2)
C(34)	36(2)	45(2)	55(2)	-7(2)	9(2)	-3(2)
C(35)	37(2)	41(2)	45(2)	1(2)	12(2)	-3(2)
C(36)	28(2)	33(2)	38(2)	2(2)	11(2)	-1(2)

C(37)	36(2)	43(2)	42(2)	0(2)	10(2)	5(2)
C(38)	49(2)	46(2)	55(2)	12(2)	12(2)	12(2)
C(39)	55(3)	35(2)	67(3)	7(2)	26(2)	2(2)
C(40)	50(2)	37(2)	57(2)	-7(2)	15(2)	-11(2)
C(41)	38(2)	36(2)	47(2)	1(2)	9(2)	0(2)

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

	x	y	z	U(eq)
H(2A)	8147	1373	-825	50
H(3A)	9181	2889	-210	50
H(5A)	8661	1909	1453	42
H(6A)	7698	263	854	43
H(9A)	6092	-1408	-2715	47
H(11A)	5338	2254	-2106	47
H(13A)	5632	2744	-957	77
H(13B)	6578	3018	-807	77
H(13C)	6285	1805	-402	77
H(14A)	5222	162	-3539	87
H(14B)	5085	1776	-3329	87
H(14C)	4504	503	-3254	87
H(15A)	7011	-2942	-2018	71
H(15B)	6933	-3061	-1291	71
H(15C)	7668	-2182	-1396	71
H(18A)	5562	-3757	183	44
H(20A)	7915	-4806	669	50
H(22A)	8804	-3517	322	78
H(22B)	8753	-1909	581	78
H(22C)	8506	-2222	-201	78
H(23A)	5025	-1697	-332	69
H(23B)	5398	-1176	-886	69
H(23C)	5619	-332	-192	69
H(24A)	6047	-6348	484	79
H(24B)	6492	-5696	1210	79

H(24C)	7000	-6578	836	79
H(26A)	9169	4145	1773	49
H(27A)	10217	5723	2345	53
H(29A)	11357	4732	1051	43
H(31A)	11759	4121	2907	42
H(32A)	12956	3045	3572	49
H(33A)	14198	3938	3584	52
H(34A)	14247	5836	2876	56
H(35A)	13056	6903	2195	50
H(37A)	10389	7813	1276	49
H(38A)	10178	10290	1234	62
H(39A)	11081	11802	2007	61
H(40A)	12194	10802	2819	59
H(41A)	12413	8329	2865	50

Table 1. Crystal data and structure refinement for Pt-NBppy.

Identification code	Pt-NBppy	
Empirical formula	C46 H45 B N2 O2 Pt	
Formula weight	863.74	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.463(5) Å	α= 111.379(6)°.
	b = 14.994(9) Å	β= 90.725(7)°.
	c = 16.501(10) Å	γ = 94.300(6)°.
Volume	1943(2) $Å^3$	
Z	2	
Density (calculated)	1.477 Mg/m^3	
Absorption coefficient	3.652 mm^{-1}	
F(000)	868	
Crystal size	0.40 x 0.03 x 0.03 mm^3	
Theta range for data collection	1.57 to 26.98°.	
Index ranges	-10<=h<=10, -18<=k<=18, -21<=l<=21	
Reflections collected	20817	
Independent reflections	8244 [R(int) = 0.1601]	
Completeness to theta = 26.98°	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8983 and 0.3229	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8244 / 0 / 478	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0996, wR2 = 0.2102	
R indices (all data)	R1 = 0.1952, wR2 = 0.2579	
Extinction coefficient	0.0054(9)	
Largest diff. peak and hole	5.635 and -4.003 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Pt(1)	1237(1)	3313(1)	4594(1)	43(1)
B(1)	-2585(18)	165(12)	2173(11)	34(4)
O(1)	2552(12)	4652(8)	5207(7)	49(3)
O(2)	243(12)	3743(7)	3704(6)	45(3)
C(1)	181(19)	1945(10)	4072(10)	42(4)
C(2)	-932(18)	1581(10)	3374(10)	44(4)
C(3)	-1372(18)	593(11)	2960(10)	39(4)
C(4)	-611(17)	-9(10)	3337(10)	40(4)
C(5)	431(19)	327(11)	4038(11)	49(4)
C(6)	820(19)	1317(11)	4430(10)	39(4)
C(7)	-2430(20)	-873(10)	1491(9)	43(4)
C(8)	-3762(18)	-1593(11)	1269(10)	43(4)
C(9)	-3580(20)	-2502(11)	681(11)	53(5)
C(10)	-2200(30)	-2809(13)	313(11)	61(5)
C(11)	-850(20)	-2084(13)	518(10)	52(5)
C(12)	-1040(19)	-1175(11)	1108(10)	45(4)
C(13)	440(20)	-453(13)	1272(13)	69(6)
C(14)	-5397(18)	-1330(12)	1640(12)	59(5)
C(15)	-2060(30)	-3810(13)	-336(13)	93(8)
C(16)	-3947(18)	800(11)	2107(11)	44(4)
C(17)	-5040(20)	1102(11)	2749(11)	50(4)
C(18)	-6371(19)	1544(12)	2637(12)	53(5)
C(19)	-6685(18)	1704(11)	1874(12)	46(4)
C(20)	-5570(20)	1454(11)	1237(10)	48(4)
C(21)	-4239(17)	1002(10)	1329(10)	38(4)
C(22)	-3050(20)	750(13)	625(10)	52(4)
C(23)	-4930(20)	904(14)	3608(11)	59(5)
C(24)	-8132(19)	2180(14)	1754(12)	62(5)
C(25)	1975(17)	1782(10)	5161(9)	35(4)
C(26)	2748(18)	1328(10)	5635(10)	41(4)
C(27)	3770(19)	1862(10)	6333(11)	49(4)

C(28)	4044(19)	2879(10)	6556(10)	42(4)
C(29)	3230(18)	3282(10)	6058(10)	41(4)
C(30)	6630(20)	3222(11)	7376(12)	48(5)
C(31)	7340(20)	2600(11)	6667(12)	48(4)
C(32)	8910(20)	2414(12)	6815(13)	56(5)
C(33)	9630(20)	2798(13)	7627(14)	65(5)
C(34)	8940(20)	3421(13)	8295(14)	66(6)
C(35)	7375(19)	3626(11)	8172(11)	47(4)
C(36)	4566(19)	4404(12)	7760(11)	45(4)
C(37)	5170(20)	5187(12)	7548(12)	54(5)
C(38)	4630(30)	6061(14)	8050(14)	71(6)
C(39)	3580(20)	6206(13)	8670(14)	68(6)
C(40)	3000(20)	5433(16)	8858(13)	72(6)
C(41)	3430(20)	4495(13)	8381(12)	57(5)
C(42)	3542(19)	6253(12)	5457(12)	57(5)
C(43)	2537(19)	5356(11)	4939(12)	47(4)
C(44)	1680(20)	5331(11)	4218(11)	46(4)
C(45)	602(18)	4596(12)	3663(11)	45(4)
C(46)	-260(20)	4723(13)	2932(12)	65(5)
N(1)	2227(14)	2774(8)	5377(8)	36(3)
N(2)	5044(15)	3455(9)	7270(8)	44(3)

Table 3. Bond lengths [Å] and angles [°] for Pt-NBppy.

Pt(1)-N(1)	1.966(12)	C(3)-C(4)	1.45(2)
Pt(1)-O(2)	2.004(10)	C(4)-C(5)	1.36(2)
Pt(1)-C(1)	2.042(15)	C(5)-C(6)	1.40(2)
Pt(1)-O(1)	2.110(10)	C(6)-C(25)	1.47(2)
B(1)-C(3)	1.55(2)	C(7)-C(12)	1.37(2)
B(1)-C(7)	1.57(2)	C(7)-C(8)	1.446(19)
B(1)-C(16)	1.58(2)	C(8)-C(9)	1.38(2)
O(1)-C(43)	1.285(18)	C(8)-C(14)	1.54(2)
O(2)-C(45)	1.320(18)	C(9)-C(10)	1.36(2)
C(1)-C(2)	1.40(2)	C(10)-C(11)	1.46(3)
C(1)-C(6)	1.41(2)	C(10)-C(15)	1.51(2)
C(2)-C(3)	1.41(2)	C(11)-C(12)	1.38(2)

C(12)-C(13)	1.55(2)	N(1)-Pt(1)-O(2)	174.6(4)
C(16)-C(17)	1.39(2)	N(1)-Pt(1)-C(1)	81.3(6)
C(16)-C(21)	1.45(2)	O(2)-Pt(1)-C(1)	94.4(5)
C(17)-C(18)	1.39(2)	N(1)-Pt(1)-O(1)	91.6(4)
C(17)-C(23)	1.55(2)	O(2)-Pt(1)-O(1)	92.5(4)
C(18)-C(19)	1.39(2)	C(1)-Pt(1)-O(1)	172.5(5)
C(19)-C(20)	1.39(2)	C(3)-B(1)-C(7)	119.5(13)
C(19)-C(24)	1.51(2)	C(3)-B(1)-C(16)	117.6(14)
C(20)-C(21)	1.39(2)	C(7)-B(1)-C(16)	122.9(13)
C(21)-C(22)	1.51(2)	C(43)-O(1)-Pt(1)	123.9(11)
C(25)-C(26)	1.39(2)	C(45)-O(2)-Pt(1)	123.0(10)
C(25)-N(1)	1.396(18)	C(2)-C(1)-C(6)	119.9(14)
C(26)-C(27)	1.38(2)	C(2)-C(1)-Pt(1)	126.9(11)
C(27)-C(28)	1.43(2)	C(6)-C(1)-Pt(1)	112.8(11)
C(28)-C(29)	1.39(2)	C(1)-C(2)-C(3)	122.5(15)
C(28)-N(2)	1.404(19)	C(2)-C(3)-C(4)	114.3(13)
C(29)-N(1)	1.348(17)	C(2)-C(3)-B(1)	123.7(14)
C(30)-C(35)	1.35(2)	C(4)-C(3)-B(1)	121.9(13)
C(30)-C(31)	1.38(2)	C(5)-C(4)-C(3)	124.6(14)
C(30)-N(2)	1.43(2)	C(4)-C(5)-C(6)	118.9(15)
C(31)-C(32)	1.41(2)	C(5)-C(6)-C(1)	119.7(15)
C(32)-C(33)	1.36(2)	C(5)-C(6)-C(25)	125.2(14)
C(33)-C(34)	1.34(2)	C(1)-C(6)-C(25)	114.9(13)
C(34)-C(35)	1.41(2)	C(12)-C(7)-C(8)	115.8(14)
C(36)-C(41)	1.39(2)	C(12)-C(7)-B(1)	123.5(14)
C(36)-C(37)	1.41(2)	C(8)-C(7)-B(1)	120.7(15)
C(36)-N(2)	1.448(19)	C(9)-C(8)-C(7)	119.4(16)
C(37)-C(38)	1.39(3)	C(9)-C(8)-C(14)	120.1(14)
C(38)-C(39)	1.33(3)	C(7)-C(8)-C(14)	120.4(14)
C(39)-C(40)	1.36(3)	C(10)-C(9)-C(8)	125.0(16)
C(40)-C(41)	1.42(2)	C(9)-C(10)-C(11)	116.1(15)
C(42)-C(43)	1.49(2)	C(9)-C(10)-C(15)	123(2)
C(43)-C(44)	1.37(2)	C(11)-C(10)-C(15)	120.3(19)
C(44)-C(45)	1.40(2)	C(12)-C(11)-C(10)	118.5(16)
C(45)-C(46)	1.48(2)	C(7)-C(12)-C(11)	125.1(15)
		C(7)-C(12)-C(13)	120.0(14)

C(11)-C(12)-C(13)	114.7(16)	C(30)-C(31)-C(32)	116.3(17)
C(17)-C(16)-C(21)	116.1(14)	C(33)-C(32)-C(31)	120.9(18)
C(17)-C(16)-B(1)	121.8(15)	C(34)-C(33)-C(32)	121.5(19)
C(21)-C(16)-B(1)	121.7(14)	C(33)-C(34)-C(35)	118.9(17)
C(16)-C(17)-C(18)	121.9(16)	C(30)-C(35)-C(34)	120.0(17)
C(16)-C(17)-C(23)	122.2(15)	C(41)-C(36)-C(37)	122.2(16)
C(18)-C(17)-C(23)	115.8(16)	C(41)-C(36)-N(2)	118.5(15)
C(17)-C(18)-C(19)	122.1(16)	C(37)-C(36)-N(2)	119.1(15)
C(20)-C(19)-C(18)	117.4(15)	C(38)-C(37)-C(36)	114.5(17)
C(20)-C(19)-C(24)	120.6(16)	C(39)-C(38)-C(37)	126.5(19)
C(18)-C(19)-C(24)	121.9(16)	C(38)-C(39)-C(40)	117.9(18)
C(19)-C(20)-C(21)	121.6(15)	C(39)-C(40)-C(41)	121(2)
C(20)-C(21)-C(16)	120.9(14)	C(36)-C(41)-C(40)	117.3(18)
C(20)-C(21)-C(22)	119.8(15)	O(1)-C(43)-C(44)	124.5(15)
C(16)-C(21)-C(22)	119.3(14)	O(1)-C(43)-C(42)	116.5(16)
C(26)-C(25)-N(1)	120.8(12)	C(44)-C(43)-C(42)	119.0(15)
C(26)-C(25)-C(6)	126.1(13)	C(43)-C(44)-C(45)	129.1(15)
N(1)-C(25)-C(6)	113.1(12)	O(2)-C(45)-C(44)	126.8(15)
C(27)-C(26)-C(25)	120.1(14)	O(2)-C(45)-C(46)	112.4(14)
C(26)-C(27)-C(28)	119.5(15)	C(44)-C(45)-C(46)	120.9(16)
C(29)-C(28)-N(2)	121.0(13)	C(29)-N(1)-C(25)	118.3(12)
C(29)-C(28)-C(27)	117.2(14)	C(29)-N(1)-Pt(1)	124.4(10)
N(2)-C(28)-C(27)	121.7(15)	C(25)-N(1)-Pt(1)	117.0(9)
N(1)-C(29)-C(28)	124.0(13)	C(28)-N(2)-C(30)	121.3(13)
C(35)-C(30)-C(31)	122.1(16)	C(28)-N(2)-C(36)	116.5(12)
C(35)-C(30)-N(2)	118.6(17)	C(30)-N(2)-C(36)	120.4(13)
C(31)-C(30)-N(2)	119.3(15)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Pt-NBppy. 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}
Pt(1)	49(1)	25(1)	51(1)	13(1)	-10(1)	-13(1)
B(1)	22(9)	37(9)	39(10)	15(8)	-19(7)	-17(7)
O(1)	51(7)	39(6)	56(7)	18(6)	-8(6)	-12(5)

O(2)	60(7)	26(5)	44(7)	11(5)	-2(5)	-10(5)
C(1)	61(11)	28(8)	38(9)	17(7)	8(8)	-6(7)
C(2)	49(10)	25(8)	47(10)	1(7)	-12(8)	-2(7)
C(3)	41(9)	38(9)	34(9)	8(7)	-3(7)	2(7)
C(4)	41(9)	24(8)	44(10)	0(7)	2(8)	-11(7)
C(5)	57(11)	31(9)	63(12)	28(8)	-17(9)	-18(8)
C(6)	53(10)	34(8)	36(9)	20(7)	6(8)	1(7)
C(7)	66(12)	31(8)	30(9)	15(7)	-7(8)	-19(8)
C(8)	43(10)	40(9)	40(10)	15(8)	-21(7)	-17(7)
C(9)	70(13)	28(9)	55(12)	15(8)	-36(10)	-14(9)
C(10)	108(17)	40(10)	30(10)	4(8)	-11(10)	23(11)
C(11)	64(12)	55(11)	32(10)	9(9)	5(9)	9(10)
C(12)	41(10)	41(9)	44(10)	9(8)	-5(8)	-15(8)
C(13)	63(13)	51(11)	83(15)	15(11)	19(11)	-9(10)
C(14)	42(10)	53(11)	85(14)	39(10)	-20(9)	-32(8)
C(15)	160(20)	33(11)	69(14)	-3(10)	-12(14)	13(13)
C(16)	31(9)	43(9)	54(11)	14(8)	4(8)	-4(7)
C(17)	46(11)	39(9)	63(12)	15(9)	-15(9)	0(8)
C(18)	39(10)	54(11)	62(13)	20(10)	8(9)	-2(8)
C(19)	35(9)	38(9)	63(12)	18(9)	-12(9)	-5(7)
C(20)	67(12)	42(10)	36(10)	17(8)	3(9)	-8(9)
C(21)	31(9)	28(8)	51(10)	12(7)	2(7)	-17(7)
C(22)	55(11)	59(11)	43(10)	20(9)	6(9)	3(9)
C(23)	66(12)	71(13)	42(11)	22(10)	4(9)	16(10)
C(24)	48(11)	68(13)	74(14)	34(11)	3(10)	-10(9)
C(25)	39(9)	35(8)	21(8)	-1(7)	-9(7)	-10(7)
C(26)	53(10)	28(8)	42(10)	15(7)	-13(8)	-11(7)
C(27)	51(10)	23(8)	64(12)	8(8)	-17(9)	-12(7)
C(28)	57(11)	20(7)	43(10)	3(7)	6(8)	-3(7)
C(29)	52(10)	18(7)	51(10)	14(7)	-12(8)	-12(7)
C(30)	55(11)	34(9)	65(12)	34(9)	-30(9)	-20(8)
C(31)	57(12)	25(8)	62(12)	18(8)	19(9)	-5(8)
C(32)	48(11)	34(9)	90(15)	26(10)	-9(10)	0(8)
C(33)	50(12)	40(10)	90(16)	10(11)	-13(11)	-13(9)
C(34)	61(13)	38(10)	80(15)	6(10)	-35(11)	-25(9)
C(35)	51(11)	27(8)	56(11)	11(8)	-22(8)	-9(7)

C(36)	39(10)	40(9)	48(11)	8(8)	-10(8)	0(7)
C(37)	58(11)	37(10)	67(12)	24(9)	-6(9)	-19(8)
C(38)	79(15)	48(12)	84(16)	23(12)	-3(13)	-7(11)
C(39)	67(14)	33(10)	87(16)	-1(10)	-11(12)	23(10)
C(40)	74(14)	71(15)	58(13)	6(11)	-11(10)	27(12)
C(41)	60(12)	47(11)	61(12)	18(10)	-15(10)	-1(9)
C(42)	47(11)	42(10)	92(15)	36(10)	17(10)	-3(8)
C(43)	37(9)	34(9)	74(13)	26(9)	15(9)	-5(7)
C(44)	64(12)	24(8)	50(11)	14(8)	11(9)	-2(8)
C(45)	37(9)	47(10)	56(11)	25(9)	-7(8)	1(8)
C(46)	56(12)	55(12)	77(14)	16(11)	2(10)	5(10)
N(1)	40(7)	23(6)	37(7)	2(6)	-11(6)	-1(5)
N(2)	45(8)	34(7)	49(8)	12(7)	-14(6)	-2(6)

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

	x	y	z	U(eq)
H(2A)	-1409	2019	3170	53
H(4A)	-858	-684	3077	48
H(5A)	887	-105	4256	59
H(9A)	-4494	-2948	520	63
H(11A)	130	-2236	252	62
H(13A)	1118	-496	1741	103
H(13B)	111	200	1441	103
H(13C)	1035	-607	739	103
H(14A)	-6132	-1911	1464	88
H(14B)	-5806	-867	1415	88
H(14C)	-5292	-1044	2277	88
H(15A)	-2907	-3974	-790	139
H(15B)	-2154	-4269	-38	139
H(15C)	-1027	-3837	-601	139
H(18A)	-7087	1742	3096	63
H(20A)	-5720	1595	726	58
H(22A)	-3531	774	90	78

H(22B)	-2742	101	515	78
H(22C)	-2115	1212	812	78
H(23A)	-5872	505	3647	89
H(23B)	-4854	1515	4106	89
H(23C)	-3979	567	3612	89
H(24A)	-8897	2171	2192	93
H(24B)	-8618	1832	1170	93
H(24C)	-7821	2847	1821	93
H(26A)	2572	652	5478	49
H(27A)	4287	1556	6662	59
H(29A)	3390	3958	6205	49
H(31A)	6808	2313	6112	57
H(32A)	9475	2017	6342	68
H(33A)	10652	2619	7719	78
H(34A)	9485	3722	8845	79
H(35A)	6846	4047	8646	56
H(37A)	5896	5123	7099	65
H(38A)	5040	6610	7939	85
H(39A)	3243	6828	8972	81
H(40A)	2291	5526	9318	86
H(41A)	2964	3951	8482	68
H(42A)	3276	6456	6071	86
H(42B)	3347	6761	5237	86
H(42C)	4664	6128	5403	86
H(44A)	1830	5889	4074	56
H(46A)	-1389	4539	2943	97
H(46B)	158	4317	2380	97
H(46C)	-107	5398	2989	97