Triaryl-Boron Functionalized Dinuclear Platinum Complexes Linked by Photoisomerizable Bpe Ligand: Luminescence and Isomerism

Supporting Information

Nan Wang, Mingfeng Hu,[†] Soren K. Mellerup,[‡] Xiang Wang,[‡] Françoise Sauriol,[‡]*

Tai Peng,[†] [†]Suning Wang[†‡]*

Table of contents

Table SA1. TD-DFT calculated electronic transition configurations for 3**B** and **4B$_{trans}$** along with their corresponding excitation energies and oscillator strengths.

Complex	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
3B	T_1	HOMO→LUMO(79%)	511.7(2.42)	—
		HOMO→LUMO+1(8%)		
		HOMO→LUMO+2(9%)		
	S_1	HOMO→LUMO(97%)	442.7(2.80)	0.0796
	S_2	HOMO-6→LUMO(2%)	374.5(3.31)	0.3201
		HOMO-3→LUMO(3%)		
		HOMO-2→LUMO(63%)		
		HOMO-1→LUMO(17%)		
		HOMO→LUMO(9%)		
	S_3	HOMO-3→LUMO(13%)	364.9(3.40)	0.0155
		HOMO-2→LUMO(15%)		
		HOMO-1→LUMO(70%)		
	S_4	HOMO-3→LUMO(77%)	359.9(3.45)	0.0765
		HOMO-2→LUMO(6%)		
		HOMO-1→LUMO(9%)		
		HOMO→LUMO+1(3%)		
	S_5	HOMO-6→LUMO(2%)	356.5(3.48)	0.1089
		HOMO-2→LUMO(7%)		
		HOMO→LUMO+1(83%)		
		HOMO→LUMO+2(3%)		

Complex	Spin State	Transition Configuration	Excitation Energy(nm, eV)	Oscillator Strength
4B$_{trans}$	T_1	HOMO→LUMO(94%)	821.7(1.51)	—
	S_1	HOMO→LUMO(99%)	765.9(1.62)	0.2242
	S_2	HOMO-1→LUMO(98%)	745.2(1.66)	0.0006
	S_3	HOMO-2→LUMO(97%)	632.9(1.96)	0.0567
	S_4	HOMO-3→LUMO(96%)	626.6(1.98)	0.0016
	S_5	HOMO-6→LUMO(34%)	567.9(2.18)	0.0007
		HOMO-4→LUMO(63%)		

Table SA2. Primary orbitals which contribute to the calculated transitions of **3B** (iso = 0.03).

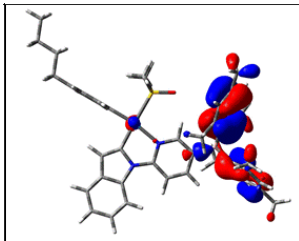
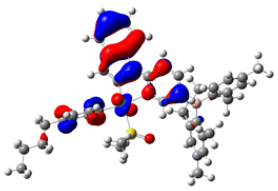
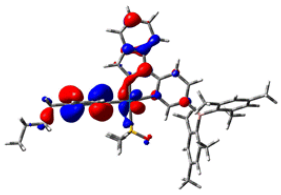
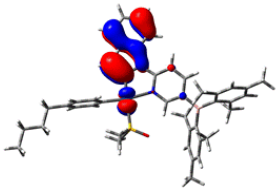
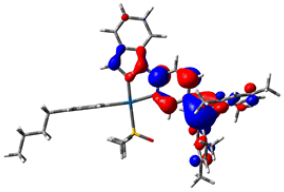
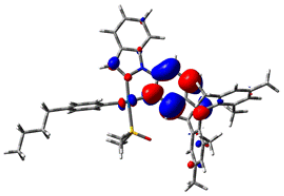
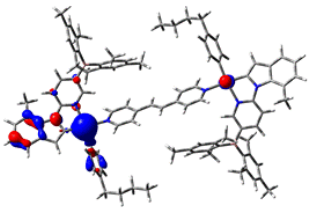
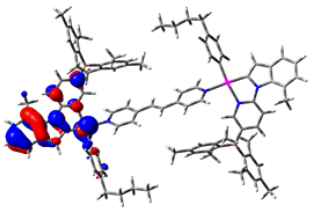
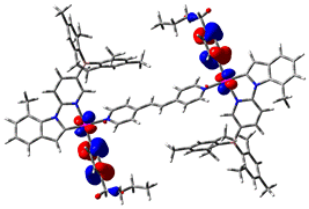
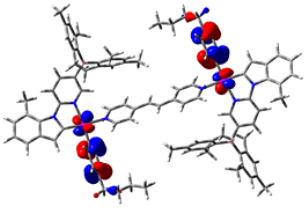
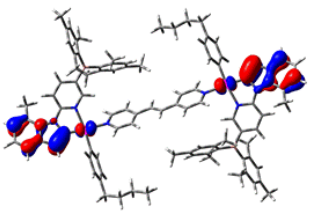
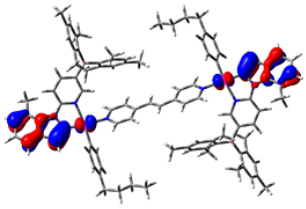
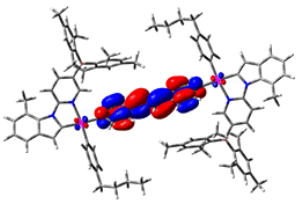
		
HOMO-3	HOMO-2	HOMO-1
		
HOMO	LUMO	LUMO+1

Table SA3. Primary orbitals which contribute to the calculated transitions of **4B** (iso = 0.03)

		
HOMO-6	HOMO-4	HOMO-3
		
HOMO-2	HOMO-1	HOMO
		
	LUMO	

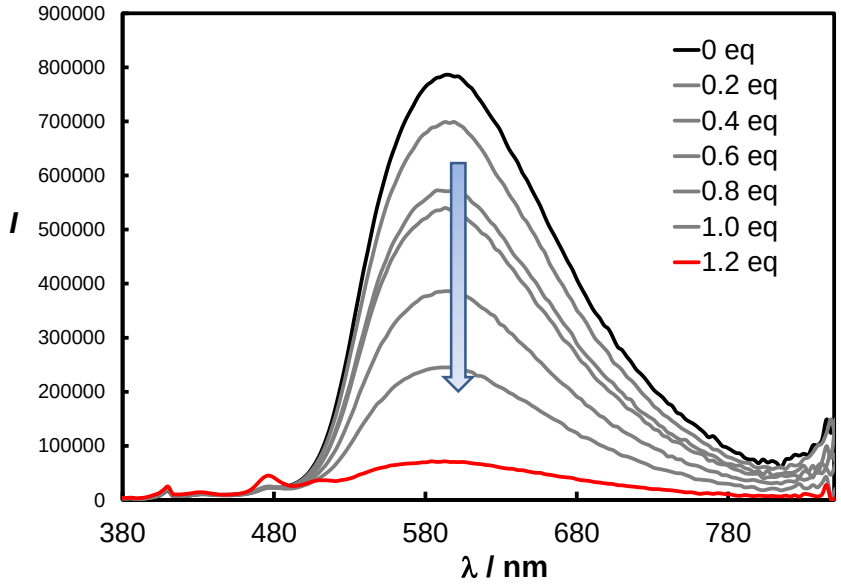


Figure SB1. Emission spectra of fluoride titration of compound **3B** in THF at room temperature under nitrogen.

SC: NMR Characterization Data

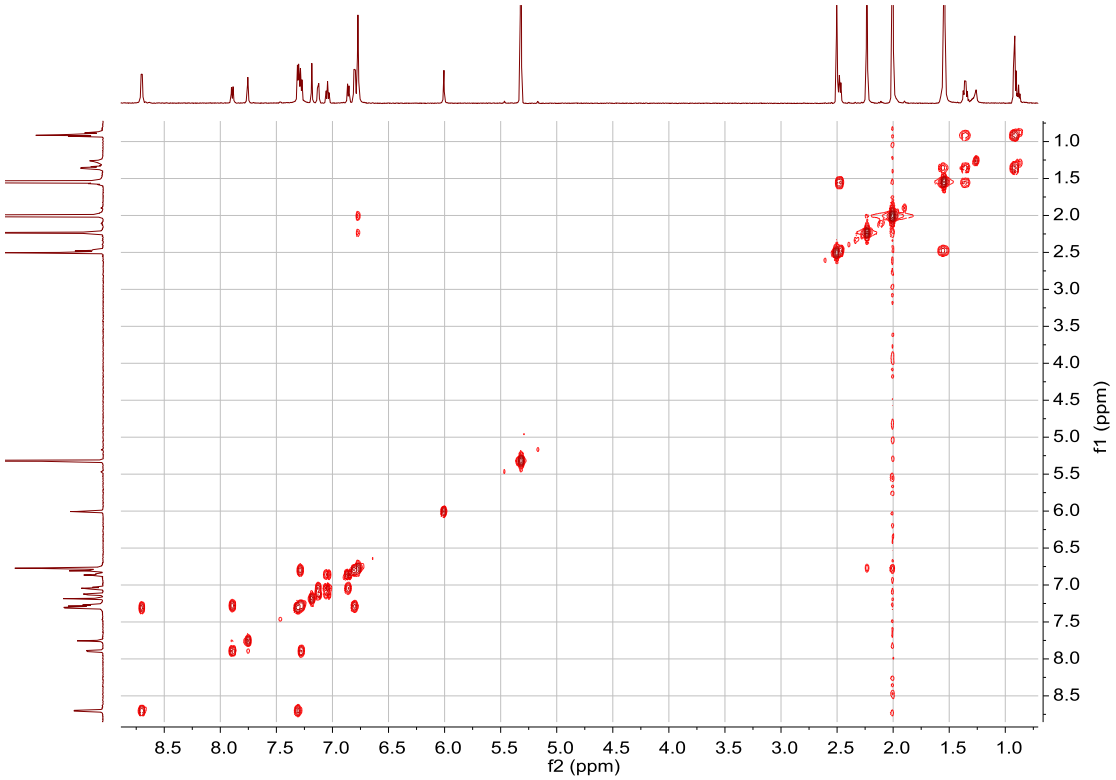


Figure SC1. The full COSY spectrum of complex **4B$_{trans}$** in CD_2Cl_2.

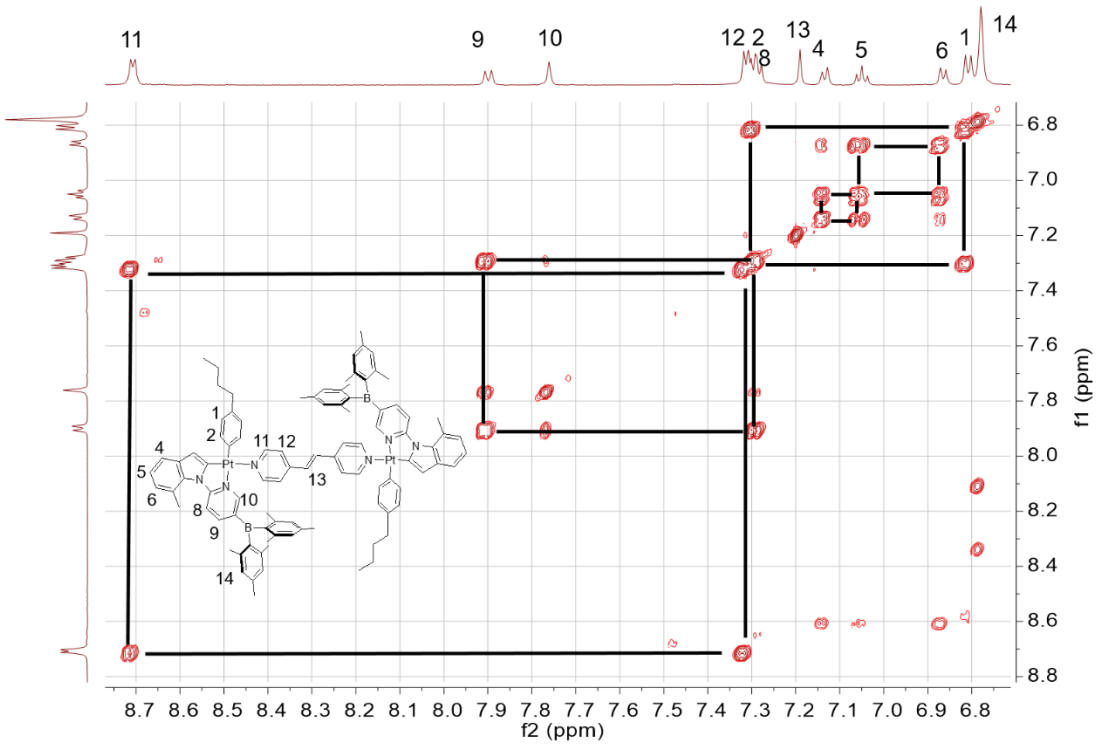


Figure SC2. The aromatic region of the COSY spectrum of **4B$_{trans}$** in CD_2Cl_2 with the 1D spectral assignment.

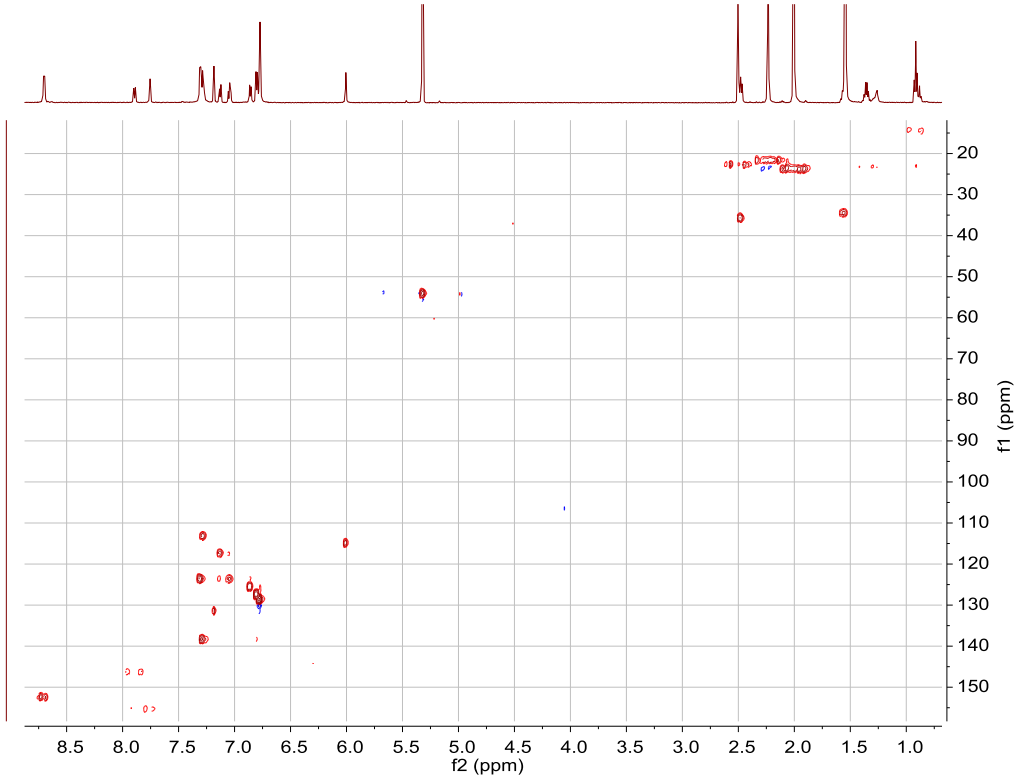


Figure SC3. HSQC spectrum of complex **4B$_{trans}$** in CD_2Cl_2

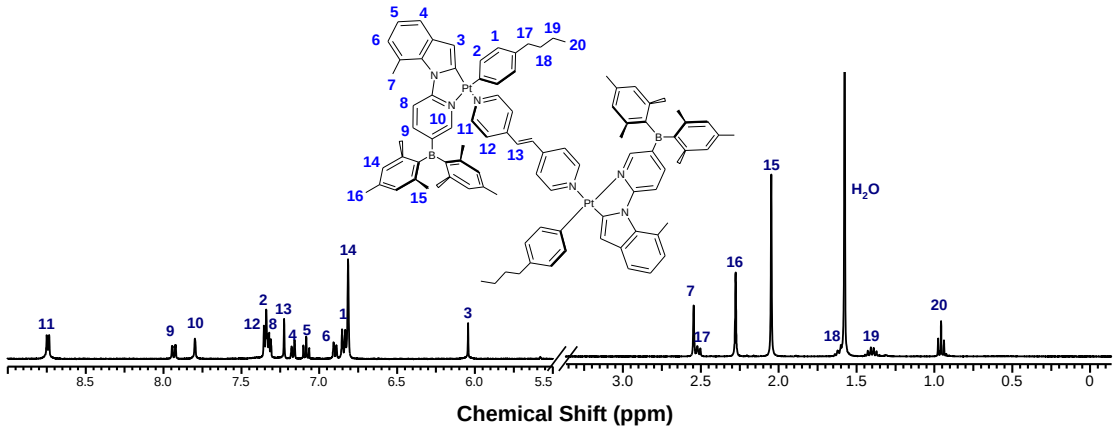


Figure SC4. Fully assigned ^{1}H NMR spectrum of **4B$_{trans}$** in CD_2Cl_2 based on 2D NMR data.

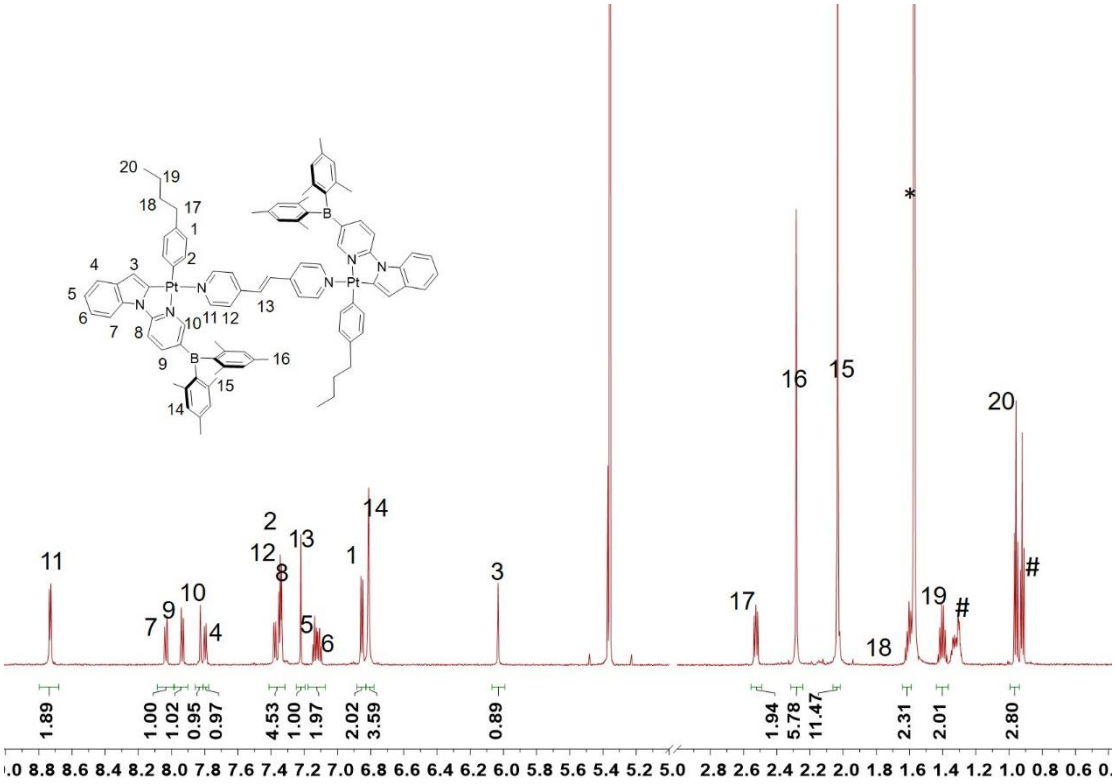


Figure SC5. Fully assigned ^{1}H NMR spectrum of **4A$_{trans}$** in CD_2Cl_2.(* H_2O; #hexane)

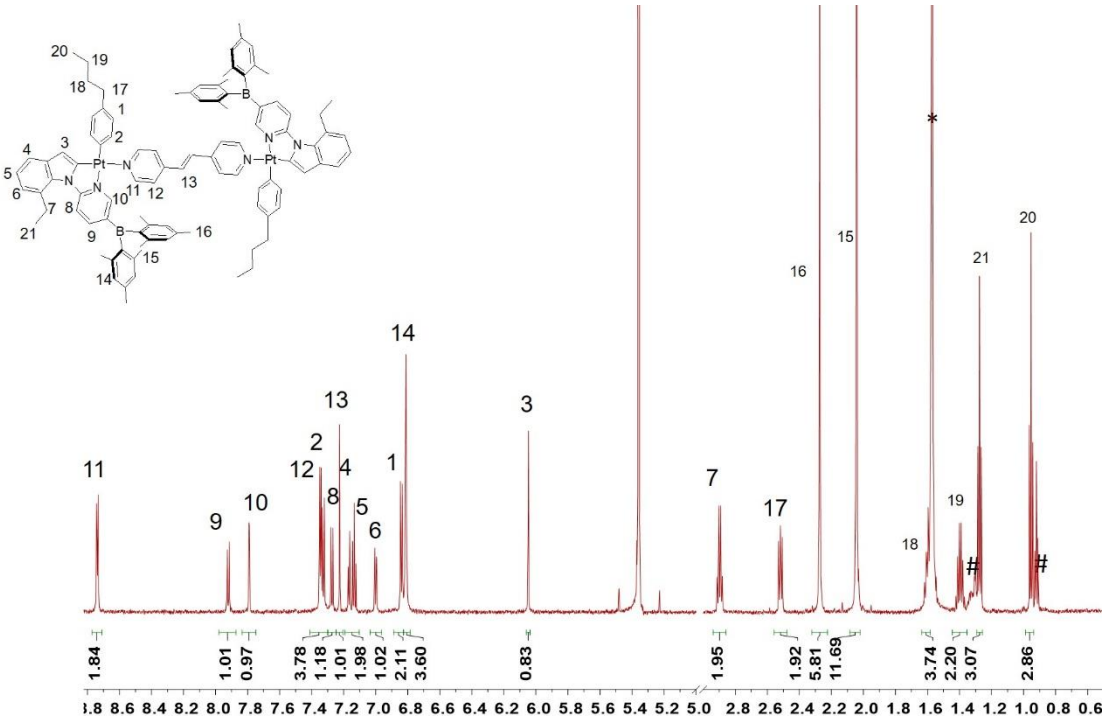


Figure SC6. Fully assigned ^{1}H NMR spectrum of **4C$_{trans}$** in CD_2Cl_2. (* H_2O; #hexane)

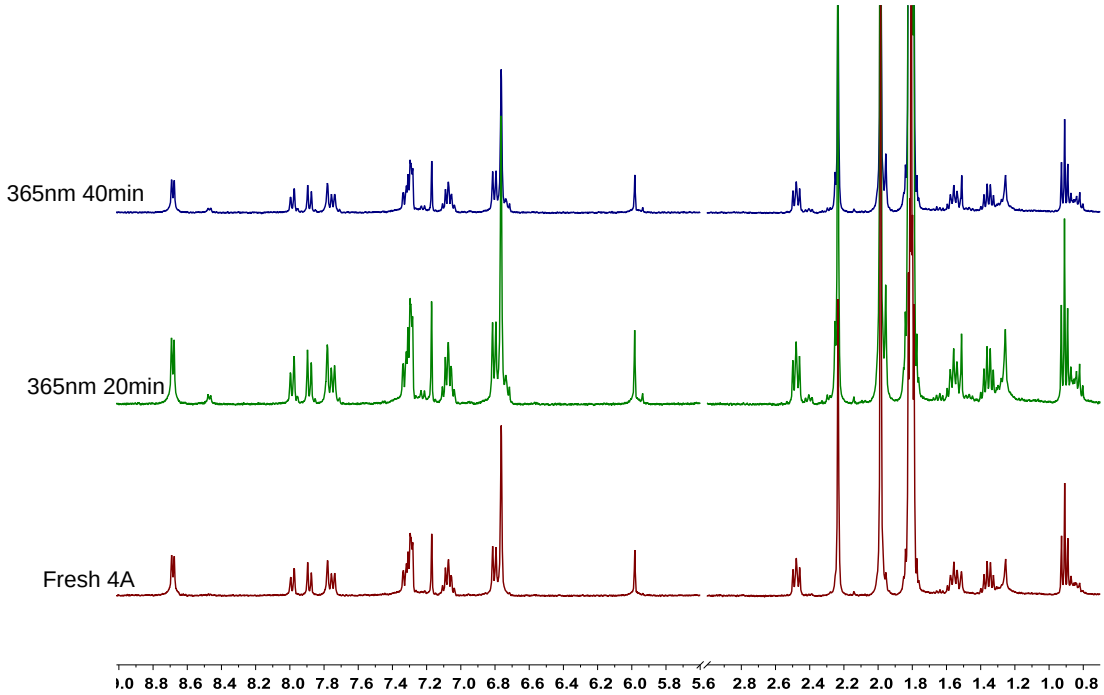


Figure SC7. ^{1}H NMR spectra of compound **4A$_{trans}$** in CD_2Cl_2 upon irradiation with UV light at 365 nm: (bottom) initial spectrum (middle and top) after 20 minutes and 40 minutes irradiation respectively.

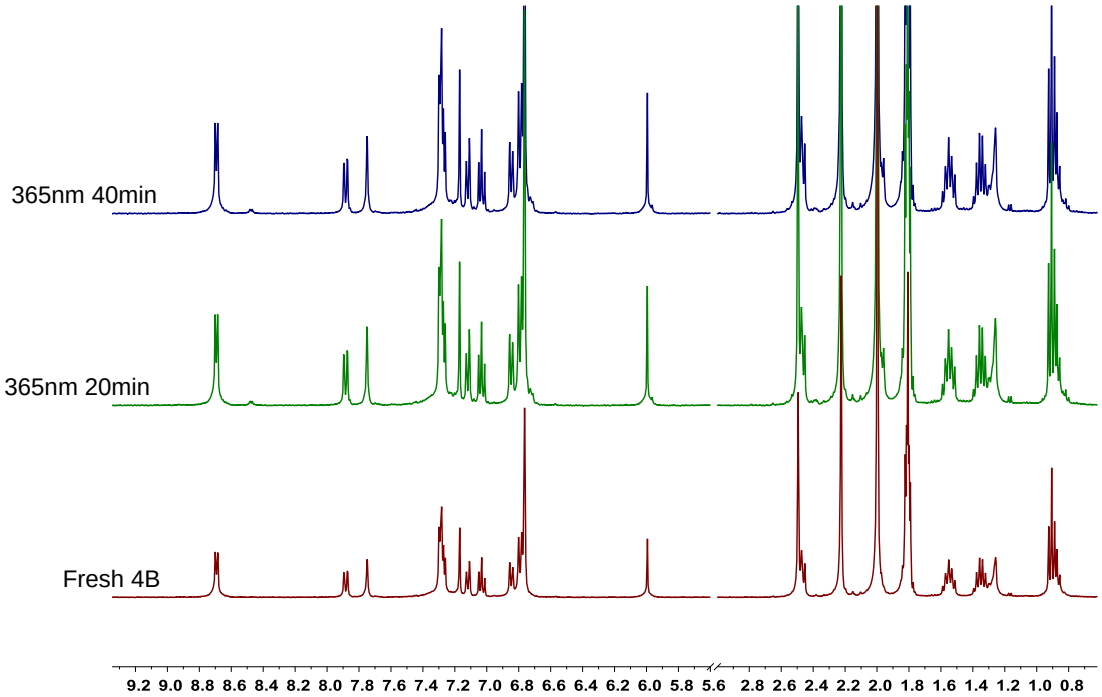


Figure SC8. ^{1}H NMR spectra of compound **4B$_{trans}$** in CD_2Cl_2 upon irradiation with UV light at 365 nm: (bottom) initial spectrum (middle and top) after 20 minutes and 40 minutes irradiation respectively.

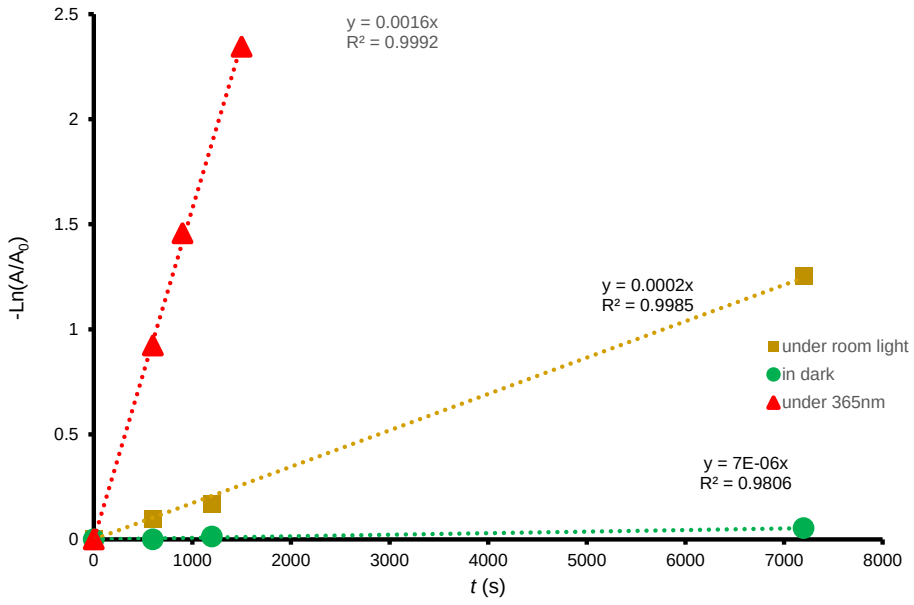


Figure SC9. Kinetic plot of the natural logarithm of the ratio of isomerized *cis*-isomer to the initial amount of *cis*-products versus time at room temperature: under ambient light (yellow square) and in dark (green circle) conditions.

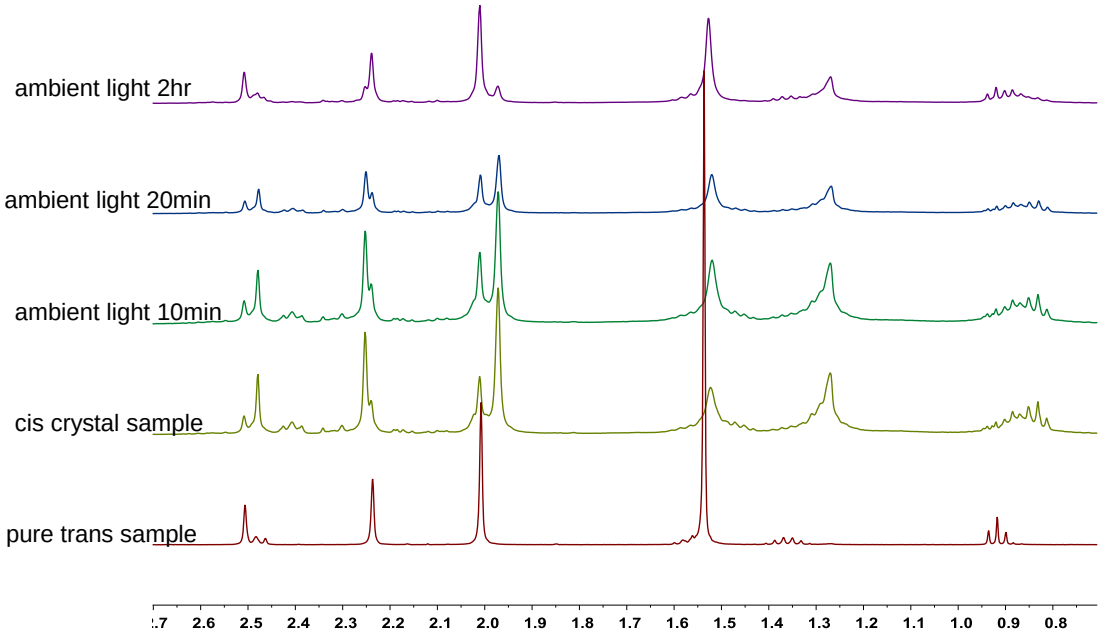


Figure SC10. ^{1}H NMR spectral changes (aliphatic region) of compound **4B** crystals (grown under ambient light) in CD_2Cl_2 upon ambient light irradiation. Fresh prepared **4B$_{trans}$** solution in CD_2Cl_2 is also included as a comparison as shown in bottom.

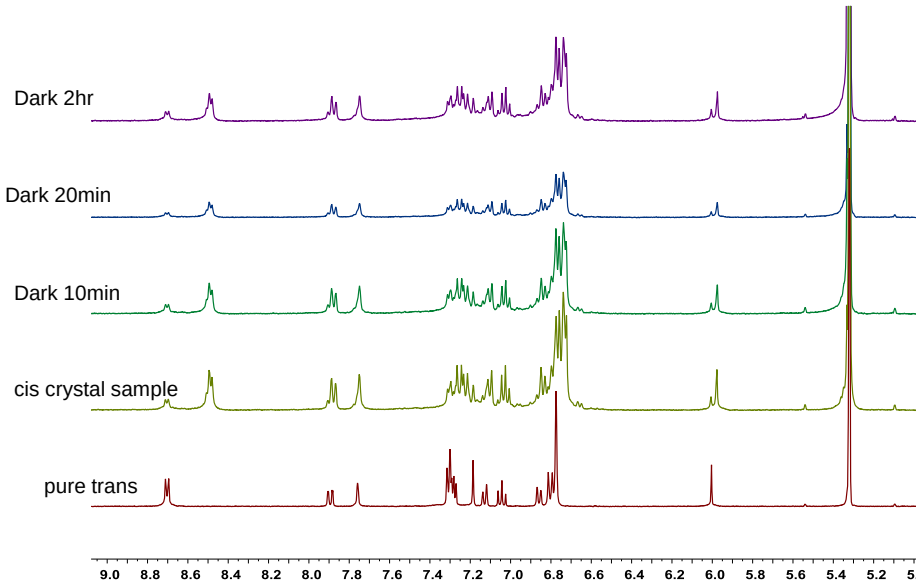


Figure SC11. ^{1}H NMR spectral changes (aromatic region) of compound **4B** crystals (grown under ambient light) in CD_2Cl_2 in dark. Fresh prepared **4B$_{trans}$** solution in CD_2Cl_2 is also included as a comparison as shown in bottom.

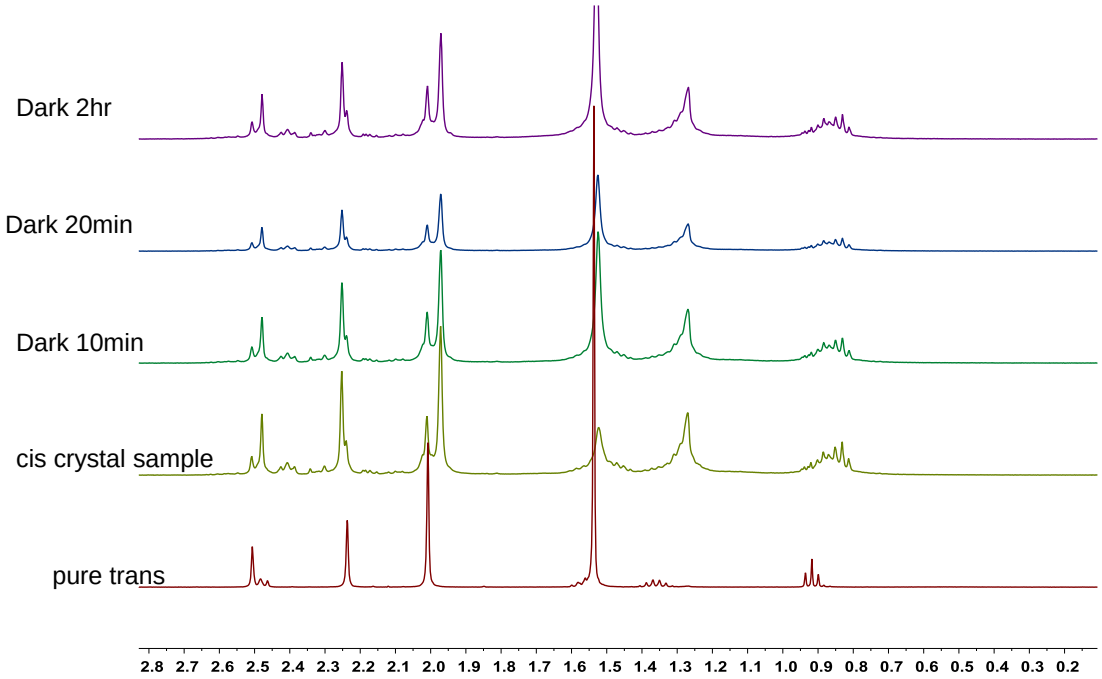


Figure SC12. ^{1}H NMR spectral changes (aliphatic region) of compound **4B** crystals (grown under ambient light) in CD_2Cl_2 in dark. Fresh prepared **4B$_{trans}$** solution in CD_2Cl_2 is also included as a comparison as shown in bottom.

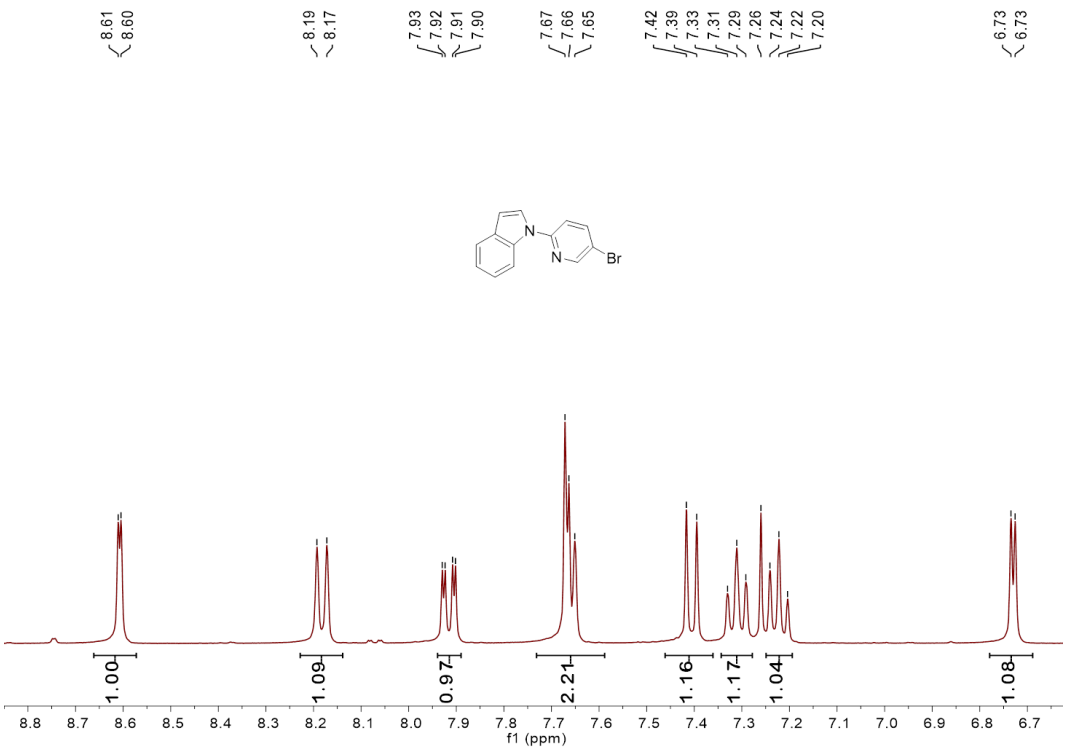


Figure SC13. ^{1}H NMR spectrum of compound **1A** in $CDCl_3$

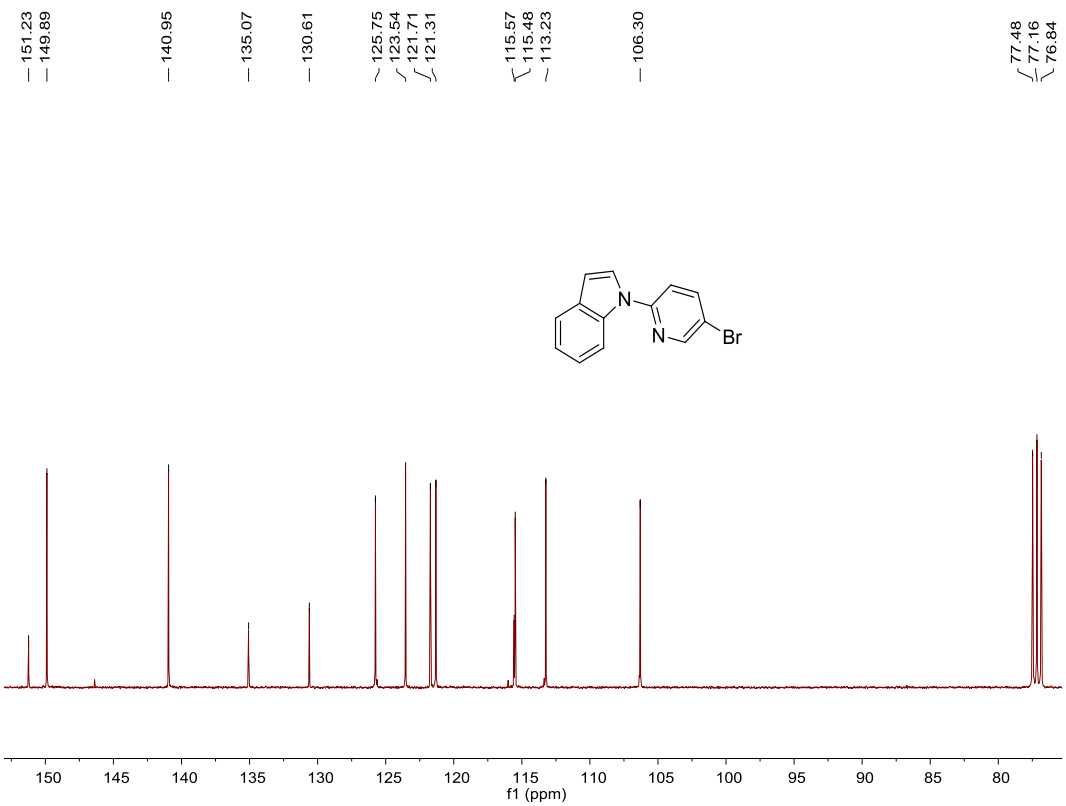


Figure SC14. ^{13}C NMR spectrum of compound **1A** in $CDCl_3$

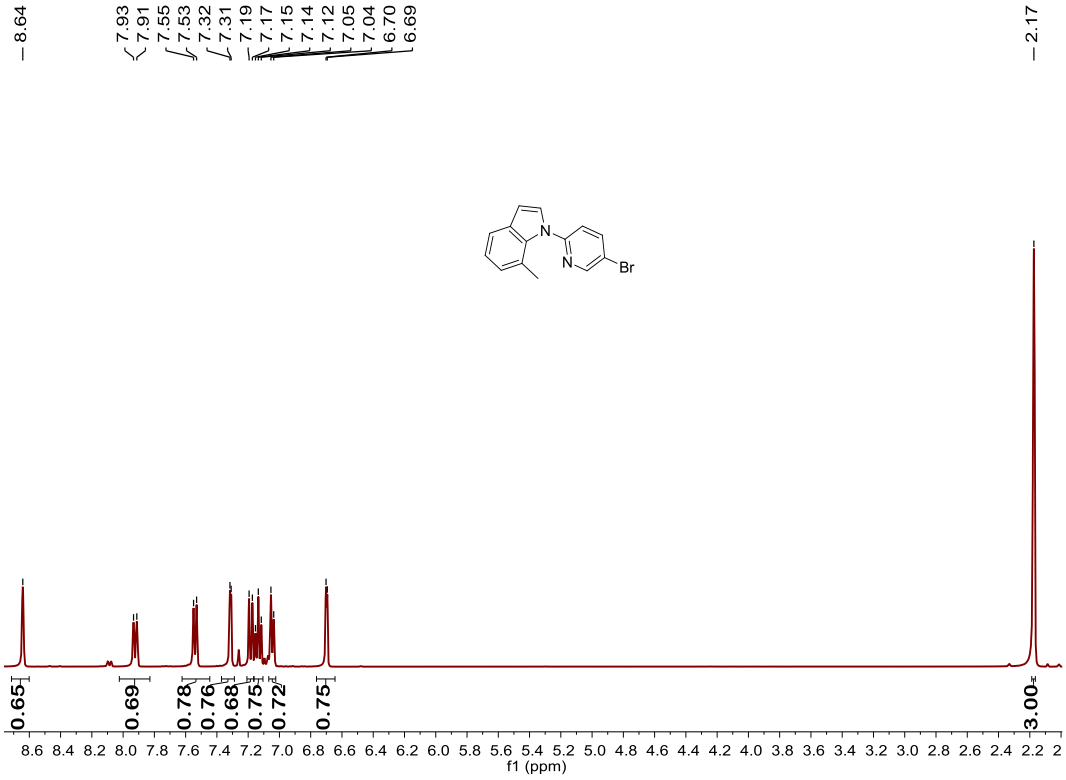


Figure SC15. ^{1}H NMR spectrum of compound **1B** in $CDCl_3$

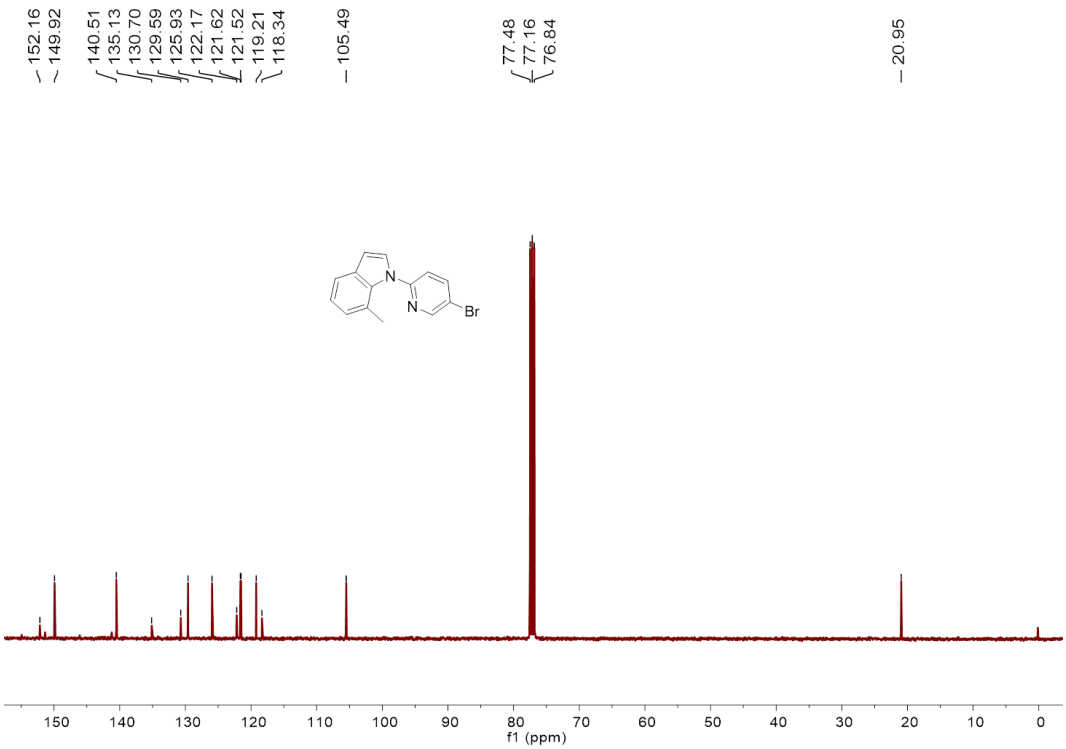


Figure SC16. ^{13}C NMR spectrum of compound **1B** in $CDCl_3$

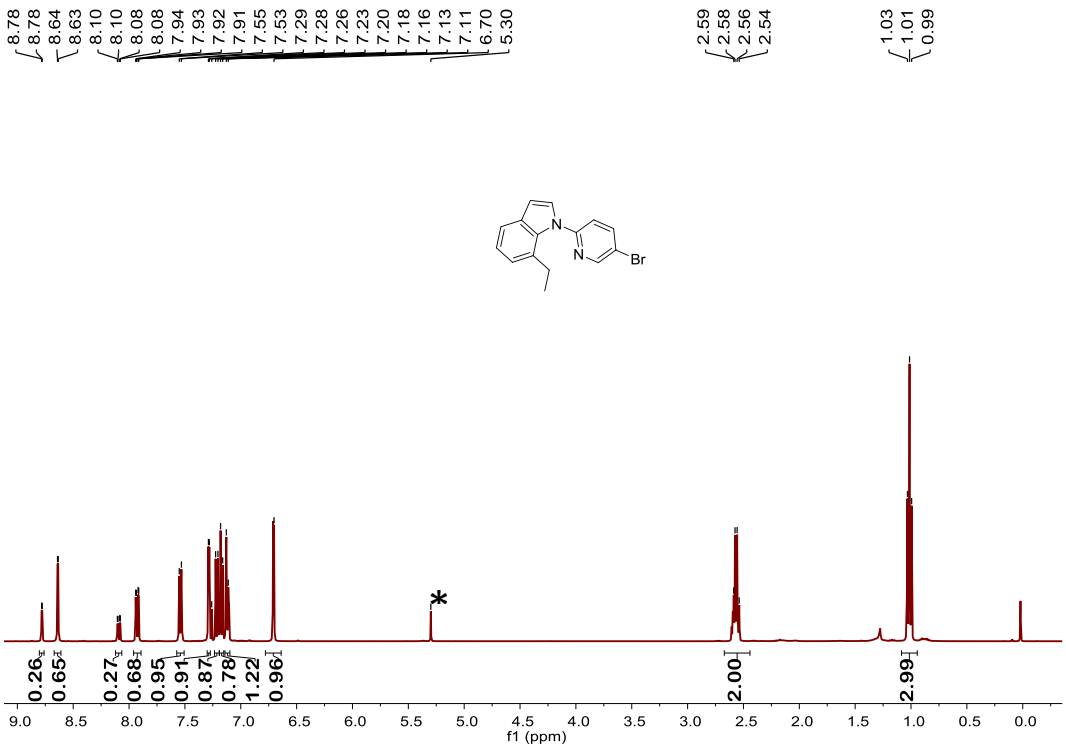


Figure SC17. ^{1}H NMR spectrum of compound **1C** in $CDCl_3$(*CH_2Cl_2)

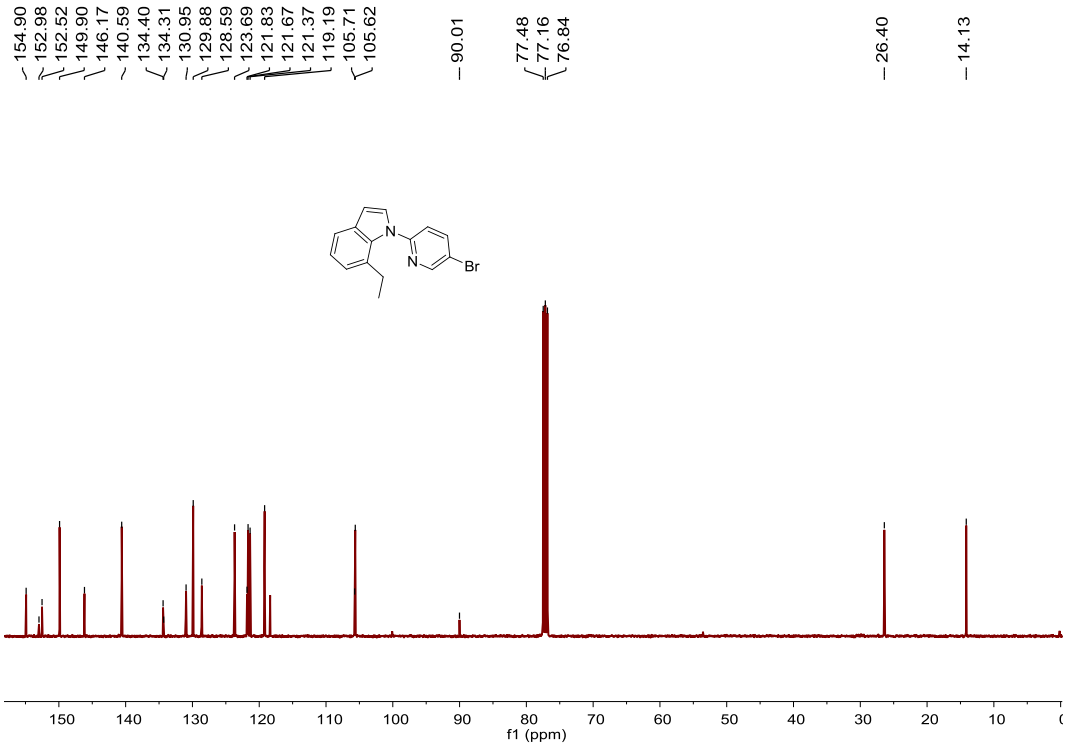


Figure SC18. ^{13}C NMR spectrum of compound **1C** in $CDCl_3$

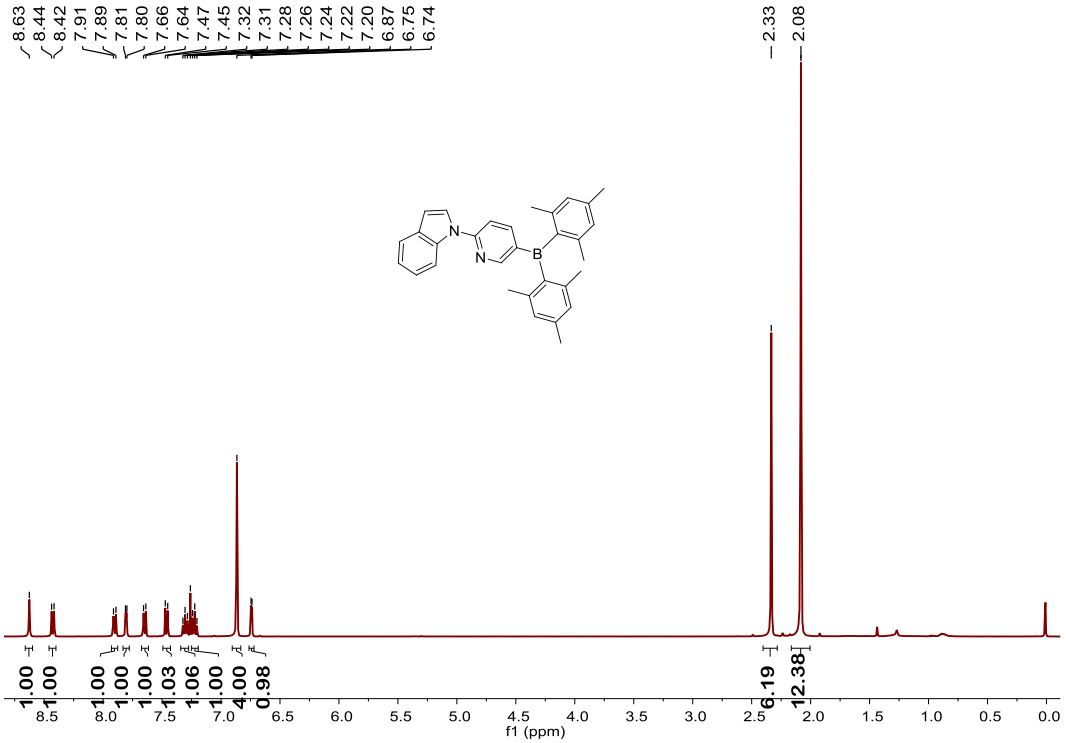


Figure SC19. ^{1}H NMR spectrum of compound **2A** in $CDCl_3$

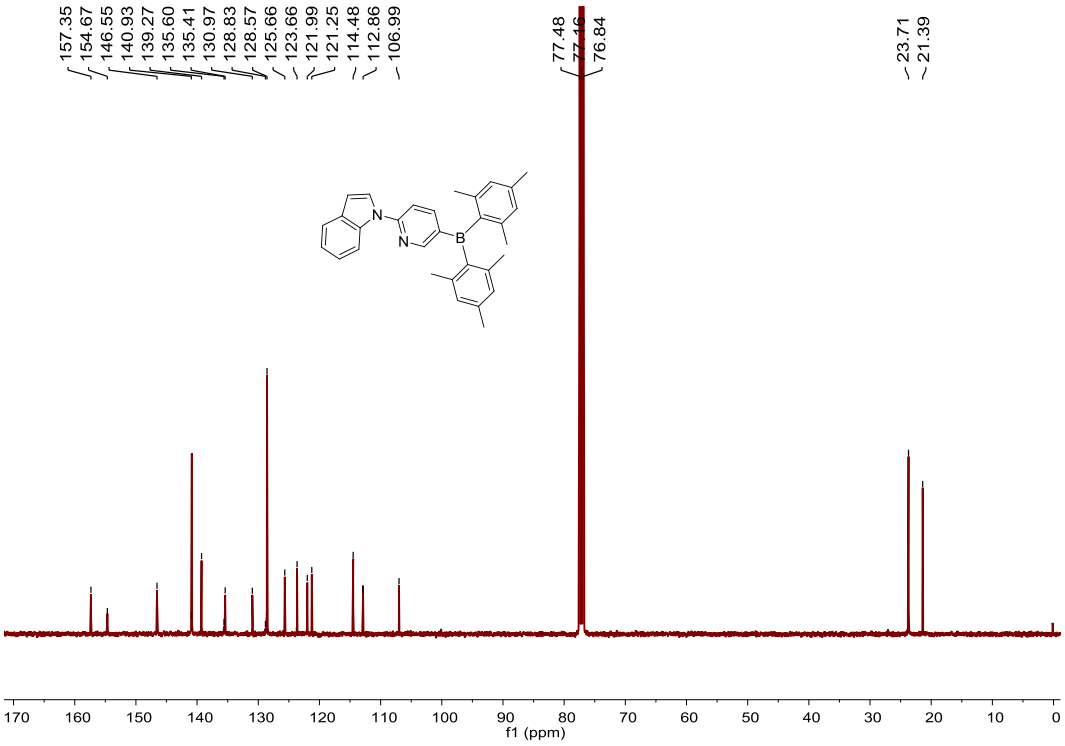


Figure SC20. ^{13}C NMR spectrum of compound **2A** in $CDCl_3$

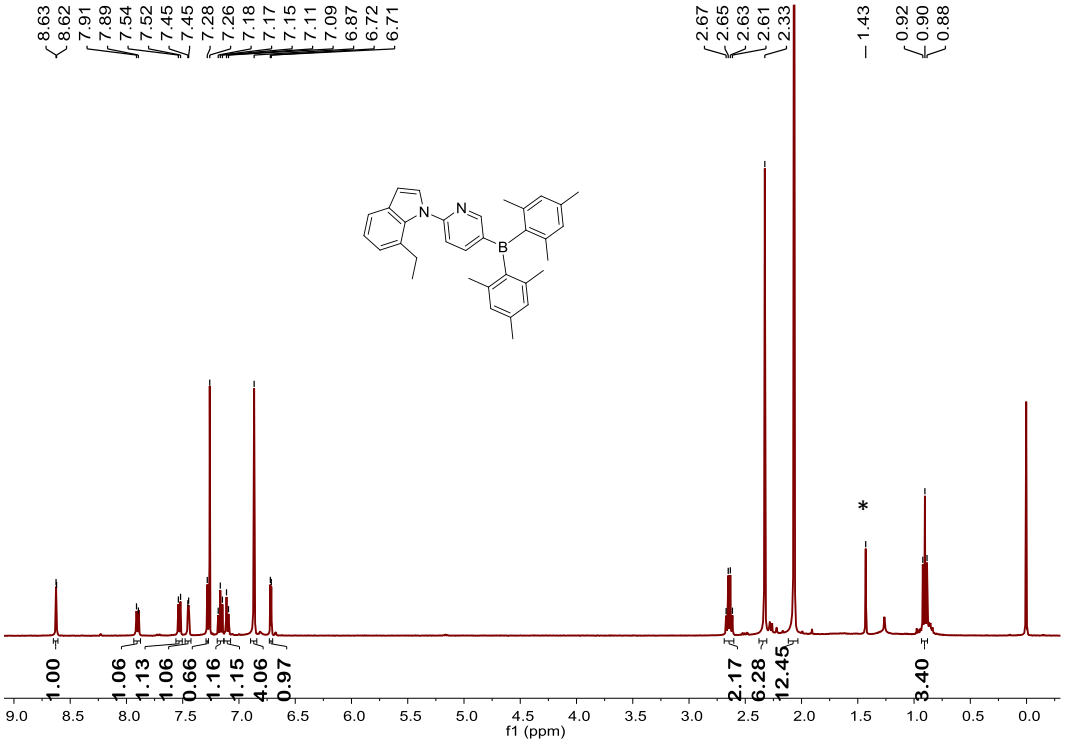


Figure SC21. ^{1}H NMR spectrum of compound **2C** in $CDCl_3$（* cyclohexane）

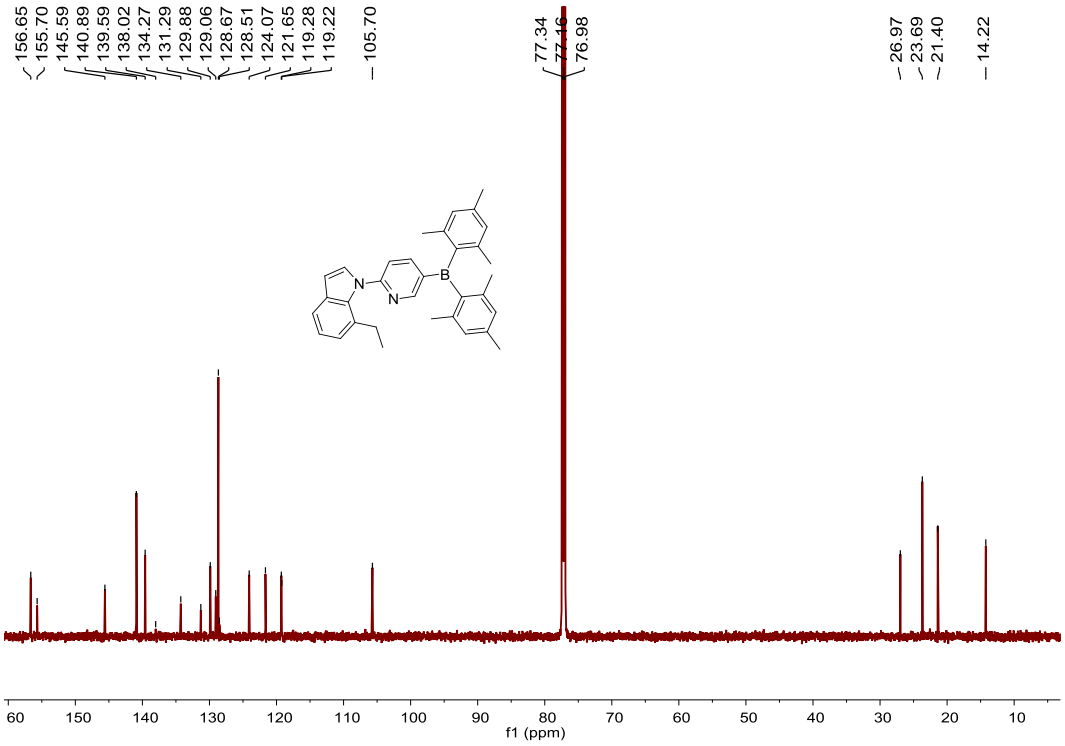


Figure SC22. ^{13}C NMR spectrum of compound **2C** in $CDCl_3$

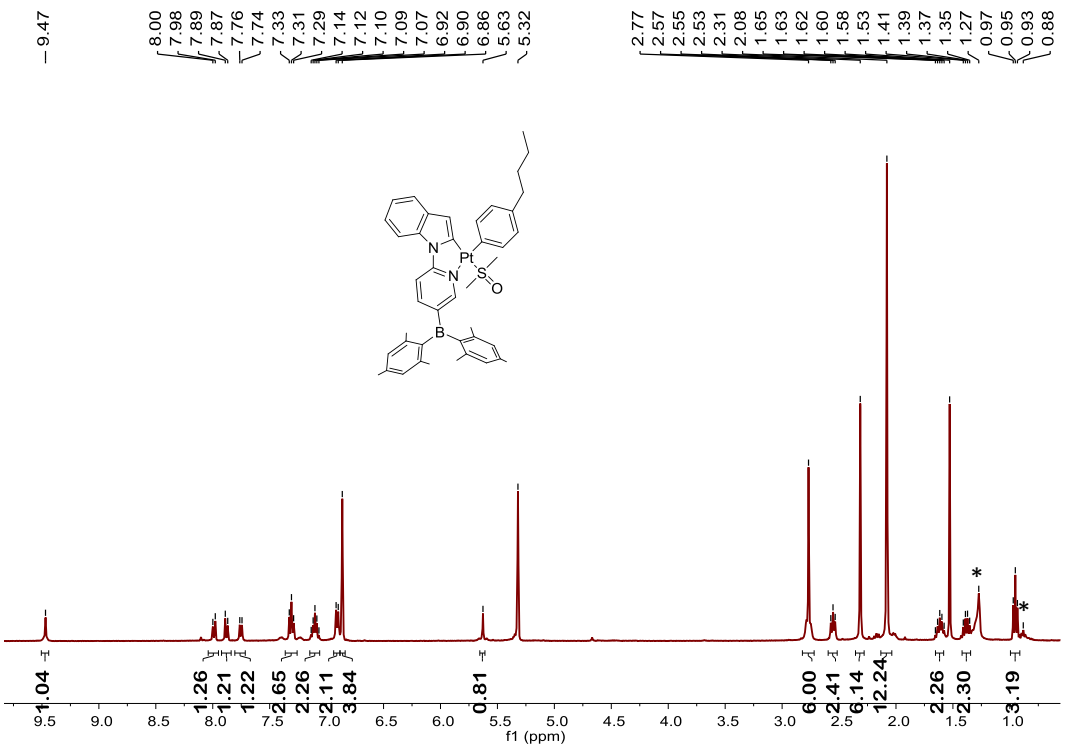


Figure SC23. ^{1}H NMR spectrum of compound **3A** in CD_2Cl_2(* grease)

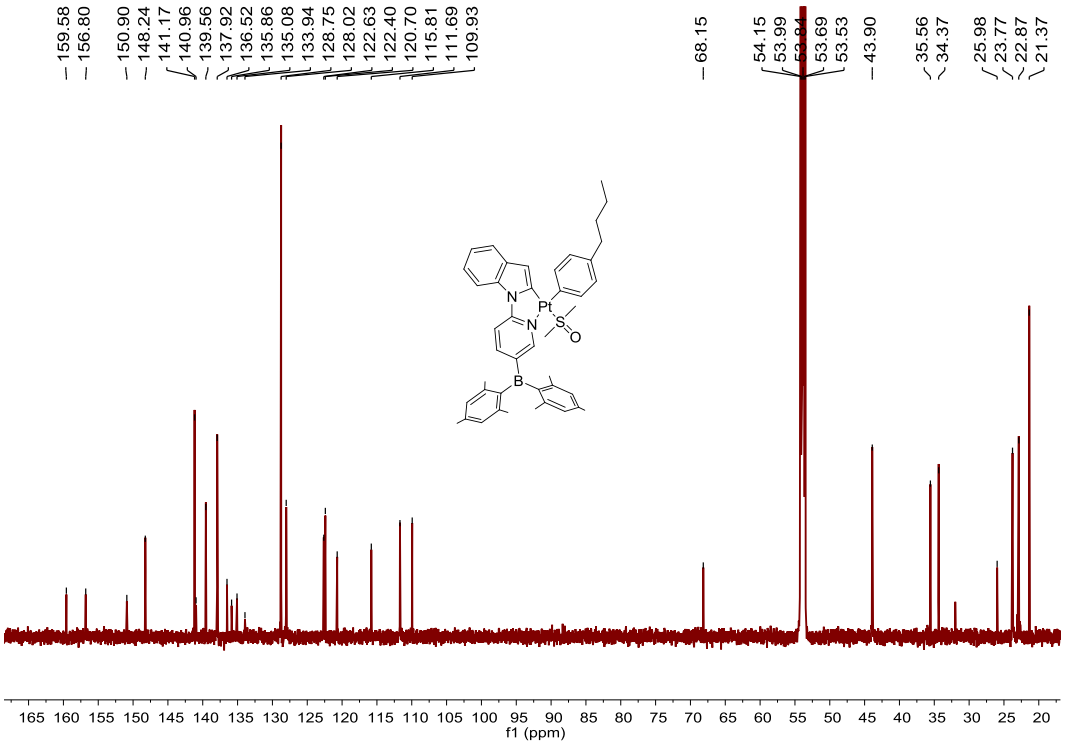


Figure SC24. ^{13}C NMR spectrum of compound **3A** in CD_2Cl_2

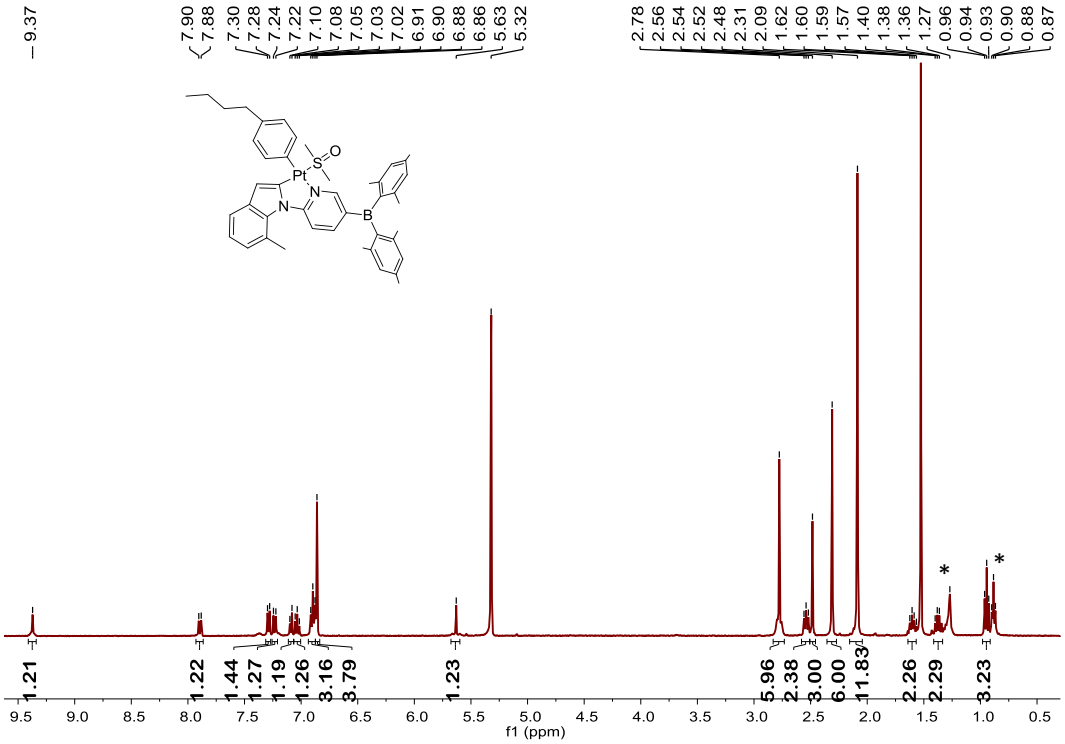


Figure SC25. ^{1}H NMR spectrum of compound **3B** in CD_2Cl_2(* n-hexane)

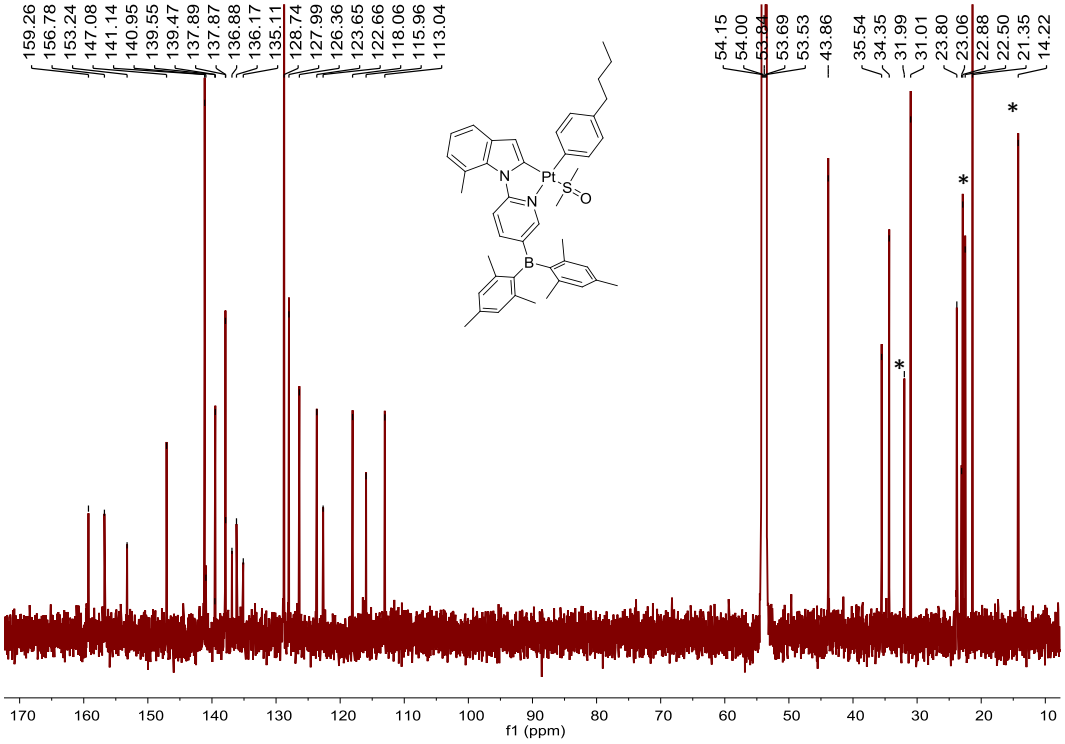


Figure SC26. ^{13}C NMR spectrum of compound **3B** in CD_2Cl_2(* n-hexane)

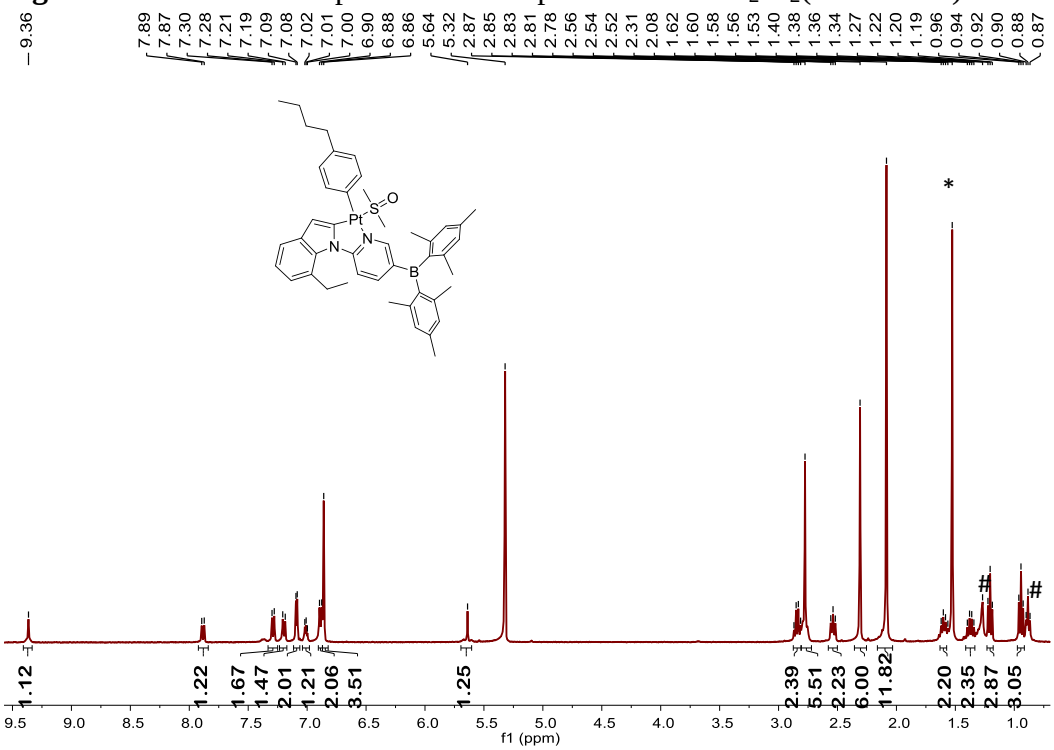


Figure SC27. ^{1}H NMR spectrum of compound **3C** in CD_2Cl_2(* H_2O , # n-hexane)

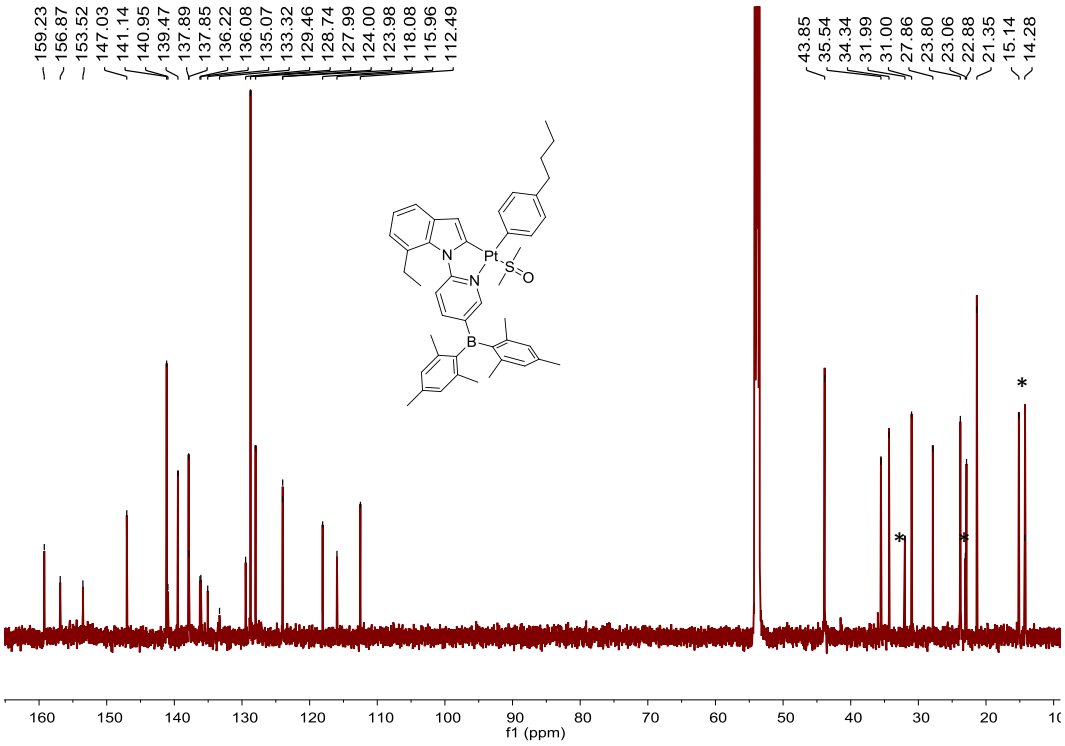


Figure SC28. ^{13}C NMR spectrum of compound **3C** in CD_2Cl_2(* n-hexane)

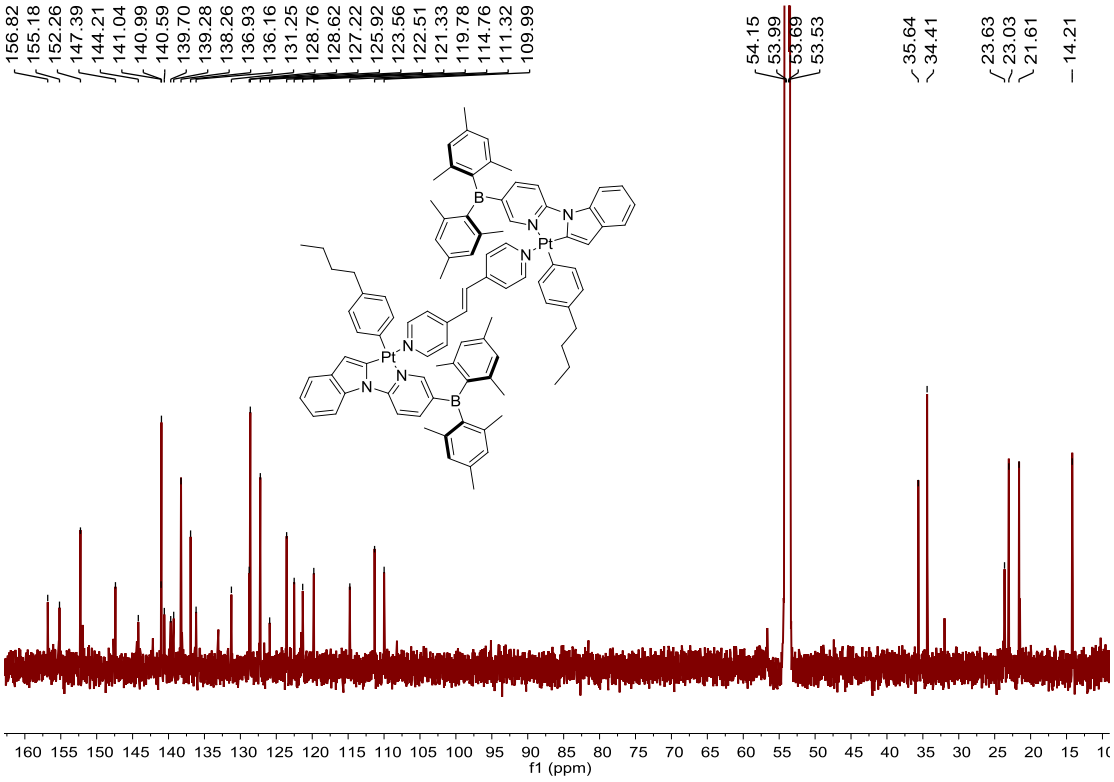


Figure SC29. ^{13}C NMR spectrum of compound **4A$_{trans}$** in CD_2Cl_2

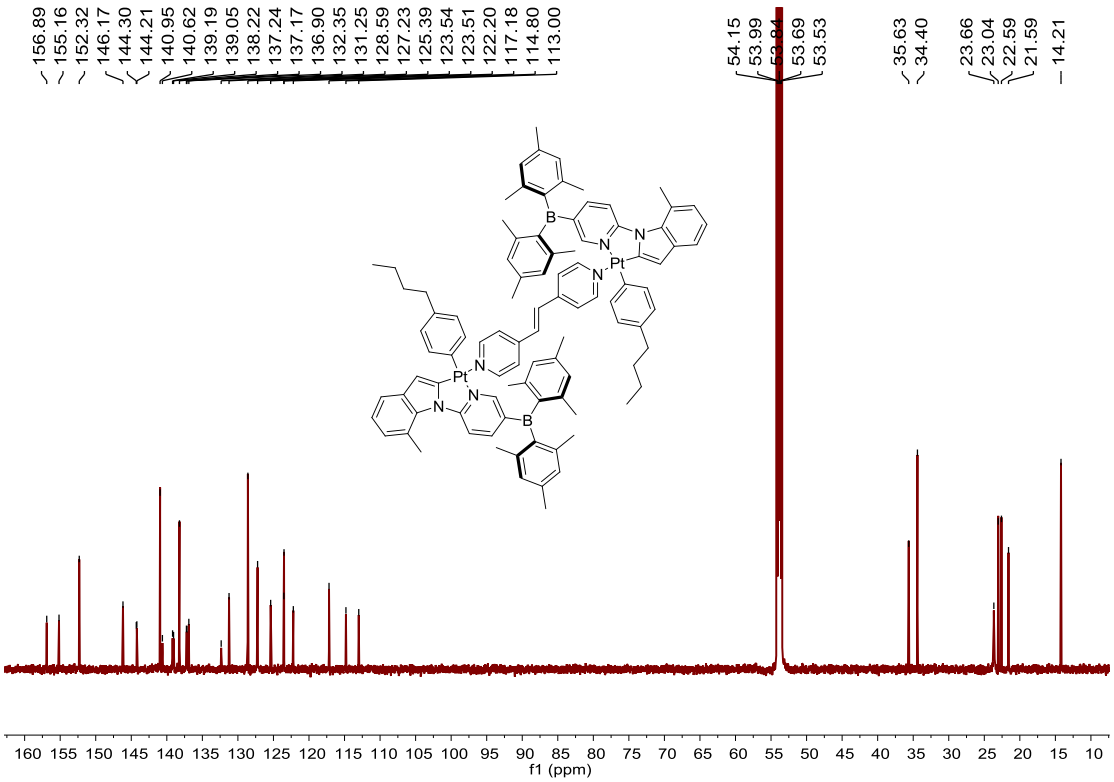


Figure SC30. ^{13}C NMR spectrum of compound **4B$_{trans}$** in CD_2Cl_2

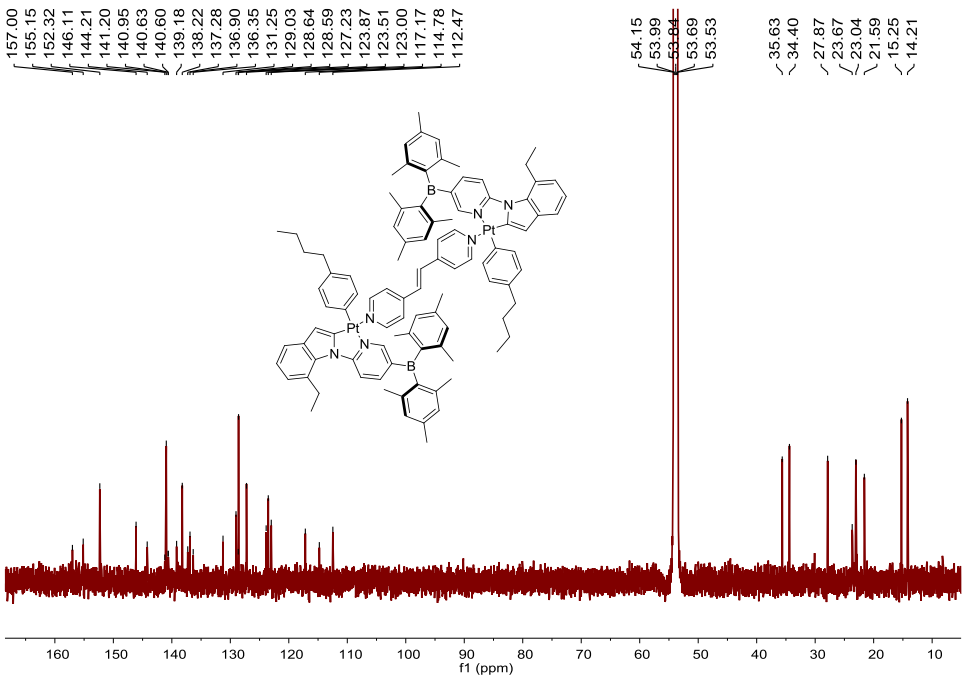


Figure SC31. ^{13}C NMR spectrum of compound **4C$_{trans}$** in CD_2Cl_2

SD. X-ray Crystallographic Data

X-ray crystallography analysis: Single crystals of **4A**, **4B** and **4B'** were obtained from CH_2Cl_2 and hexanes by slow evaporation of the solvent. The crystals were mounted on glass fibers and the data were collected on a Bruker Apex II single-crystal X-ray diffractometer with graphite-monochromated Mo Kα radiation operating at 50 kV and 30 mA (T = 180 K). Data were processed using the Bruker SHELXTL software package (version 6.10) and corrected for absorption effects. Due to the weak reflections and easily solvent lost, the structural refinement of crystal **4B'$_{cis}$** was not completed because of the limited amount of data. The crystal data given here is only for information.

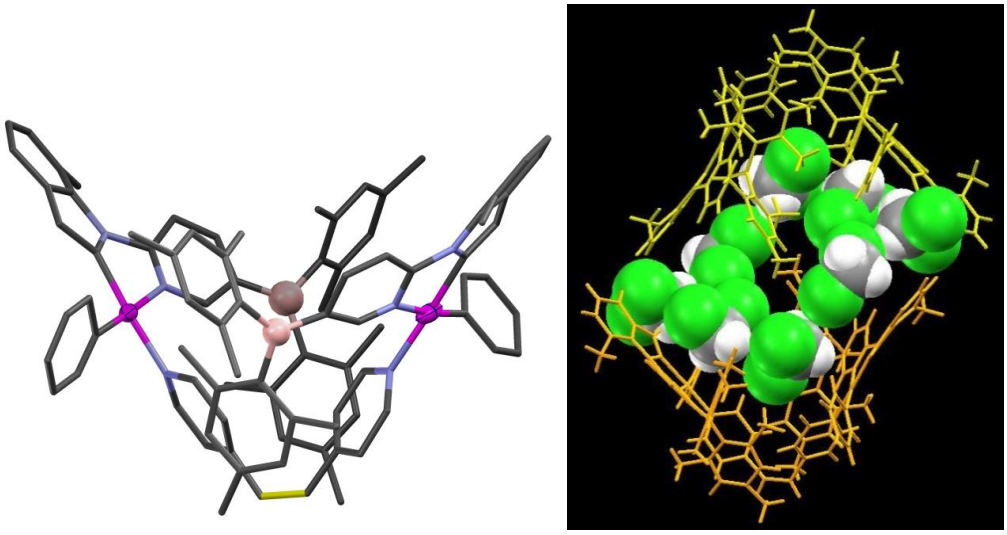


Figure SD1. Crystal structure of **4B'$_{cis}$** based on the incompletely refined structural data of **4B'$_{cis}$.**

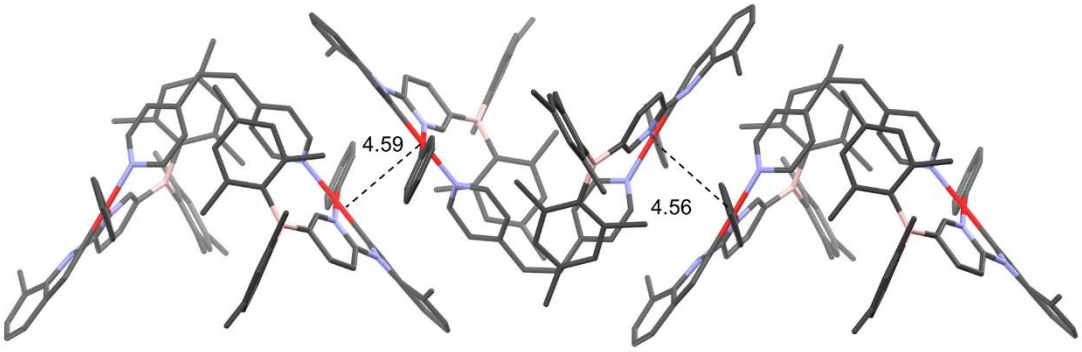


Figure SD2. A diagram showing intermolecular stacking interactions and short Pt···Pt contact distances in the crystal lattice of **4B'$_{cis}$.**

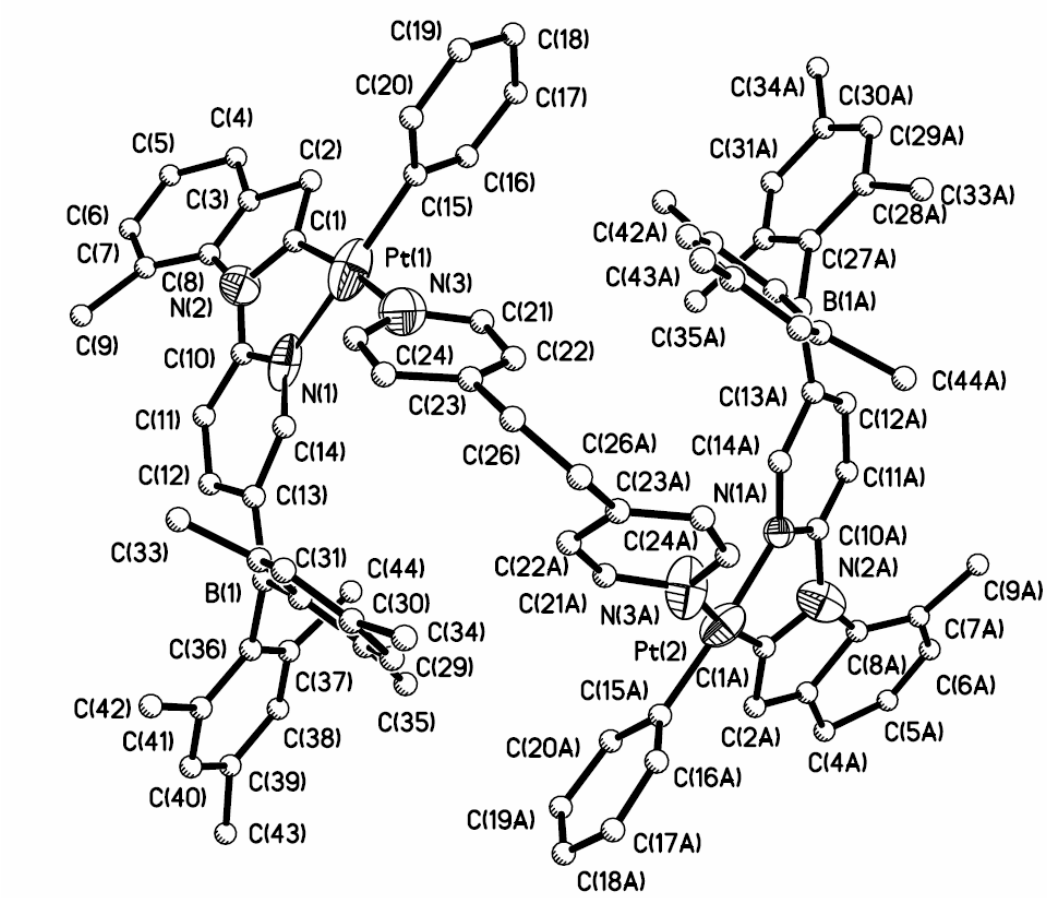


Figure SD3. A diagram showing the structure of **4B'** with labeling schemes.

Table SD1. Crystal data and structure refinement for compound**4B'**.

Identification code	compound4B'	
Empirical formula	C20 H0 B Cl2 N4 Pt0.50	
Formula weight	475.49	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.282(9) Å	α= 96.468(9)°.
	b = 18.736(13) Å	β= 105.118(8)°.
	c = 21.222(15) Å	γ = 106.587(9)°.
Volume	4785(6) $Å^3$	
Z	8	
Density (calculated)	1.320 Mg/m^3	
Absorption coefficient	3.188 mm^{-1}	
F(000)	1808	
Crystal size	0.020 x 0.020 x 0.020 mm^3	
Theta range for data collection	1.675 to 27.505°	
Index ranges	-17<=h<=17, -23<=k<=23, -27<=l<=27	
Reflections collected	55187	
Independent reflections	21131 [R(int) = 0.2740]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.939 and 0.939	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21131 / 6 / 443	
Goodness-of-fit on F^2	0.682	
Final R indices [I>2sigma(I)]	R1 = 0.0955, wR2 = 0.2066	
R indices (all data)	R1 = 0.3354, wR2 = 0.2652	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.066 and -0.950 e. $Å^{-3}$	

Table SD2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound4B'. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	-9937(1)	-14724(1)	-8905(1)	79(1)
Pt(2)	-6792(1)	-10518(1)	-5655(1)	56(1)
N(1)	-10781(11)	-14073(10)	-9360(7)	57(5)
N(1A)	-6669(10)	-11316(7)	-5120(7)	31(4)
N(2A)	-7237(12)	-10689(9)	-4431(8)	61(5)
N(2)	-12281(13)	-15173(10)	-9608(8)	56(5)
N(3A)	-6008(11)	-10793(9)	-6281(7)	64(5)
N(3)	-8378(13)	-13950(9)	-8666(9)	68(5)
C(1A)	-7494(14)	-10350(10)	-4975(9)	38(5)
C(1)	-11550(20)	-15415(15)	-9199(12)	82(8)
C(2A)	-8131(13)	-9856(9)	-4857(8)	37(5)
C(2)	-12008(16)	-16114(12)	-8995(9)	70(7)
C(3)	-13185(19)	-16242(13)	-9427(11)	71(7)
C(3A)	-8264(17)	-9931(12)	-4216(11)	67(6)
C(4)	-14070(20)	-16910(14)	-9454(12)	93(8)
C(4A)	-8770(15)	-9569(11)	-3822(14)	77(8)
C(5A)	-8560(20)	-9759(13)	-3134(15)	97(10)
C(5)	-15121(19)	-17020(14)	-9984(12)	78(8)
C(6A)	-7950(17)	-10152(12)	-2854(12)	60(7)
C(6)	-15105(19)	-16472(15)	-10369(12)	79(9)
C(7A)	-7402(19)	-10436(13)	-3207(12)	74(7)
C(7)	-14226(15)	-15858(14)	-10299(10)	69(8)
C(8)	-13299(19)	-15743(12)	-9784(11)	58(6)
C(8A)	-7626(15)	-10401(10)	-3866(10)	50(5)
C(9A)	-6510(20)	-10757(14)	-2845(12)	113(10)
C(9)	-14387(16)	-15439(14)	-10888(10)	93(9)
C(10A)	-6956(17)	-11353(13)	-4600(11)	68(7)

C(10)	-11867(19)	-14421(14)	-9615(11)	65(7)
C(11)	-12600(20)	-13993(13)	-9856(11)	87(8)
C(11A)	-7170(17)	-11922(12)	-4219(11)	79(7)
C(12A)	-6812(18)	-12522(14)	-4394(12)	99(8)
C(12)	-12200(18)	-13253(13)	-9823(10)	83(7)
C(13A)	-6343(16)	-12556(12)	-4912(10)	69(6)
C(13)	-11016(18)	-12875(13)	-9562(10)	71(7)
C(14A)	-6300(15)	-11916(11)	-5261(10)	62(6)
C(14)	-10513(17)	-13415(13)	-9380(9)	53(6)
C(15A)	-7051(15)	-9787(10)	-6208(9)	46(5)
C(15)	-9244(15)	-15426(10)	-8438(9)	47(5)
C(16)	-9470(20)	-15656(14)	-7885(13)	110(9)
C(16A)	-6401(16)	-9302(11)	-6401(9)	60(6)
C(17)	-8930(20)	-16110(15)	-7531(14)	126(10)
C(17A)	-6509(17)	-8755(12)	-6788(10)	72(7)
C(18A)	-7545(18)	-8704(12)	-7014(10)	79(7)
C(18)	-8230(20)	-16440(15)	-7740(14)	124(10)
C(19A)	-8390(20)	-9209(16)	-6859(13)	127(10)
C(19)	-7980(20)	-16210(15)	-8307(13)	117(10)
C(20)	-8545(19)	-15754(14)	-8634(12)	102(9)
C(20A)	-8190(19)	-9742(13)	-6415(11)	87(8)
C(21A)	-6605(14)	-11080(9)	-6959(9)	41(5)
C(21)	-7668(17)	-13665(11)	-8038(11)	73(7)
C(22)	-6640(18)	-13093(12)	-7943(12)	76(7)
C(22A)	-6145(16)	-11331(10)	-7441(10)	59(6)
C(23A)	-5130(19)	-11396(12)	-7235(12)	78(7)
C(23)	-6320(20)	-12864(14)	-8410(14)	98(8)
C(24A)	-4529(16)	-11161(10)	-6569(10)	60(6)
C(24)	-6973(18)	-13087(13)	-9076(12)	88(8)
C(25A)	-5051(15)	-10897(10)	-6151(9)	45(5)
C(25)	-8029(18)	-13647(13)	-9158(12)	85(8)
C(26A)	-4600(20)	-11621(14)	-7744(11)	96(8)
C(26)	-5170(20)	-12262(15)	-8253(13)	115(9)
C(27A)	-6624(19)	-14059(8)	-4930(9)	104(9)
C(28A)	-5942(11)	-14411(12)	-4571(9)	101(8)
C(29A)	-6398(19)	-15079(12)	-4372(8)	146(11)

C(30A)	-7540(20)	-15395(9)	-4532(10)	153(12)
C(31A)	-8221(12)	-15043(13)	-4891(10)	179(14)
C(32A)	-7764(17)	-14375(13)	-5090(8)	131(10)
C(27)	-9312(12)	-11605(12)	-9345(11)	88(8)
C(28)	-8620(20)	-10996(12)	-8832(9)	180(14)
C(29)	-7505(19)	-10697(10)	-8782(10)	205(16)
C(30)	-7091(12)	-11007(14)	-9243(13)	144(11)
C(31)	-7790(20)	-11615(14)	-9755(11)	192(15)
C(32)	-8898(19)	-11915(9)	-9806(8)	161(13)
C(33A)	-4710(18)	-14031(14)	-4357(12)	118(9)
C(33)	-9405(18)	-12429(12)	-10479(10)	97(8)
C(34A)	-8170(20)	-16173(15)	-4434(14)	159(12)
C(34)	-5828(19)	-10623(15)	-9001(13)	136
C(35A)	-8650(20)	-13995(16)	-5575(14)	163(13)
C(35)	-9100(20)	-10663(15)	-8332(12)	135(11)
C(36A)	-5331(14)	-13292(11)	-5688(8)	85(7)
C(37A)	-5645(12)	-13811(8)	-6283(10)	122(10)
C(38A)	-4988(18)	-13715(10)	-6702(7)	135(11)
C(39A)	-4017(16)	-13100(13)	-6525(9)	165(13)
C(40A)	-3704(11)	-12581(9)	-5930(10)	143(11)
C(41A)	-4361(15)	-12677(9)	-5512(7)	92(8)
C(36)	-11412(12)	-11493(10)	-9463(10)	110(9)
C(37)	-11979(13)	-11513(8)	-8997(8)	84(7)
C(38)	-12621(11)	-11046(9)	-8975(7)	74(7)
C(39)	-12695(12)	-10559(8)	-9420(9)	87(8)
C(40)	-12127(16)	-10538(10)	-9886(8)	160(12)
C(41)	-11486(14)	-11005(12)	-9908(8)	184(15)
C(42)	-10880(20)	-11004(17)	-10456(14)	163(12)
C(42A)	-6780(20)	-14491(17)	-6472(15)	169(13)
C(43)	-13220(30)	-9950(20)	-9358(18)	231(18)
C(43A)	-3280(30)	-13090(20)	-7029(17)	225(18)
C(44)	-11786(18)	-12000(13)	-8423(11)	100(8)
C(44A)	-3742(19)	-12095(13)	-4806(11)	113(9)
B(1A)	-6099(18)	-13295(15)	-5173(13)	71(9)
B(1)	-10630(30)	-12013(18)	-9484(15)	98(10)

Table SD3. Bond lengths [Å] and angles [°] for compound **4B**'$_{cis}$.

Pt(1)-C(15)	2.018(19)
Pt(1)-N(1)	2.039(18)
Pt(1)-C(1)	2.05(3)
Pt(1)-N(3)	2.054(16)
Pt(2)-C(15A)	1.947(19)
Pt(2)-C(1A)	1.954(17)
Pt(2)-N(1A)	1.994(14)
Pt(2)-N(3A)	1.996(14)
N(1)-C(14)	1.19(2)
N(1)-C(10)	1.33(2)
N(1A)-C(10A)	1.26(2)
N(1A)-C(14A)	1.38(2)
N(2A)-C(1A)	1.39(2)
N(2A)-C(10A)	1.43(2)
N(2A)-C(8A)	1.53(2)
N(2)-C(1)	1.34(3)
N(2)-C(10)	1.36(2)
N(2)-C(8)	1.39(2)
N(3A)-C(25A)	1.304(19)
N(3A)-C(21A)	1.405(19)
N(3)-C(21)	1.36(2)
N(3)-C(25)	1.36(2)
C(1A)-C(2A)	1.46(2)
C(1)-C(2)	1.44(3)
C(2A)-C(3A)	1.43(2)
C(2)-C(3)	1.53(3)
C(3)-C(8)	1.28(2)
C(3)-C(4)	1.43(3)
C(3A)-C(4A)	1.43(3)
C(3A)-C(8A)	1.51(2)
C(4)-C(5)	1.49(3)
C(4A)-C(5A)	1.52(3)
C(5A)-C(6A)	1.32(3)
C(5)-C(6)	1.38(3)

C(6A)-C(7A)	1.34(3)
C(6)-C(7)	1.35(3)
C(7A)-C(8A)	1.36(2)
C(7A)-C(9A)	1.55(3)
C(7)-C(8)	1.36(3)
C(7)-C(9)	1.55(3)
C(10A)-C(11A)	1.42(3)
C(10)-C(11)	1.46(3)
C(11)-C(12)	1.32(3)
C(11A)-C(12A)	1.39(3)
C(12A)-C(13A)	1.40(3)
C(12)-C(13)	1.45(3)
C(13A)-C(14A)	1.48(2)
C(13A)-B(1A)	1.58(3)
C(13)-C(14)	1.40(2)
C(13)-B(1)	1.52(3)
C(15A)-C(16A)	1.25(2)
C(15A)-C(20A)	1.49(2)
C(15)-C(20)	1.37(3)
C(15)-C(16)	1.37(3)
C(16)-C(17)	1.42(3)
C(16A)-C(17A)	1.40(2)
C(17)-C(18)	1.39(3)
C(17A)-C(18A)	1.37(2)
C(18A)-C(19A)	1.38(3)
C(18)-C(19)	1.41(3)
C(19A)-C(20A)	1.48(3)
C(19)-C(20)	1.41(3)
C(21A)-C(22A)	1.42(2)
C(21)-C(22)	1.42(3)
C(22)-C(23)	1.25(3)
C(22A)-C(23A)	1.35(2)
C(23A)-C(24A)	1.38(2)
C(23A)-C(26A)	1.52(3)
C(23)-C(24)	1.39(3)
C(23)-C(26)	1.54(3)

C(24A)-C(25A)	1.39(2)
C(24)-C(25)	1.45(3)
C(26A)-C(26)	1.39(3)
C(27A)-C(28A)	1.3900
C(27A)-C(32A)	1.3900
C(27A)-B(1A)	1.61(3)
C(28A)-C(29A)	1.3900
C(28A)-C(33A)	1.50(2)
C(29A)-C(30A)	1.3900
C(30A)-C(31A)	1.3900
C(30A)-C(34A)	1.53(2)
C(31A)-C(32A)	1.3900
C(32A)-C(35A)	1.72(2)
C(27)-C(28)	1.3900
C(27)-C(32)	1.3900
C(27)-B(1)	1.63(3)
C(28)-C(29)	1.3900
C(28)-C(35)	1.54(2)
C(29)-C(30)	1.3900
C(30)-C(31)	1.3900
C(30)-C(34)	1.54(2)
C(31)-C(32)	1.3900
C(32)-C(33)	1.50(2)
C(36A)-C(37A)	1.3900
C(36A)-C(41A)	1.3900
C(36A)-B(1A)	1.68(3)
C(37A)-C(38A)	1.3900
C(37A)-C(42A)	1.59(3)
C(38A)-C(39A)	1.3900
C(39A)-C(40A)	1.3900
C(39A)-C(43A)	1.63(3)
C(40A)-C(41A)	1.3900
C(41A)-C(44A)	1.61(2)
C(36)-C(37)	1.3900
C(36)-C(41)	1.3900
C(36)-B(1)	1.62(3)

C(37)-C(38)	1.3900
C(37)-C(44)	1.61(2)
C(38)-C(39)	1.3900
C(39)-C(40)	1.3900
C(39)-C(43)	1.51(4)
C(40)-C(41)	1.3900
C(41)-C(42)	1.58(3)

C(15)-Pt(1)-N(1)	174.2(7)
C(15)-Pt(1)-C(1)	98.3(10)
N(1)-Pt(1)-C(1)	76.4(9)
C(15)-Pt(1)-N(3)	87.9(7)
N(1)-Pt(1)-N(3)	97.4(6)
C(1)-Pt(1)-N(3)	173.8(10)
C(15A)-Pt(2)-C(1A)	103.4(8)
C(15A)-Pt(2)-N(1A)	175.0(7)
C(1A)-Pt(2)-N(1A)	74.8(7)
C(15A)-Pt(2)-N(3A)	84.5(7)
C(1A)-Pt(2)-N(3A)	172.1(8)
N(1A)-Pt(2)-N(3A)	97.3(6)
C(14)-N(1)-C(10)	113(2)
C(14)-N(1)-Pt(1)	132.3(15)
C(10)-N(1)-Pt(1)	114.3(16)
C(10A)-N(1A)-C(14A)	109.6(18)
C(10A)-N(1A)-Pt(2)	123.8(15)
C(14A)-N(1A)-Pt(2)	126.6(13)
C(1A)-N(2A)-C(10A)	112.0(17)
C(1A)-N(2A)-C(8A)	111.6(15)
C(10A)-N(2A)-C(8A)	133.8(18)
C(1)-N(2)-C(10)	112(2)
C(1)-N(2)-C(8)	107(2)
C(10)-N(2)-C(8)	138.9(19)
C(25A)-N(3A)-C(21A)	110.1(15)
C(25A)-N(3A)-Pt(2)	129.4(13)
C(21A)-N(3A)-Pt(2)	118.9(11)
C(21)-N(3)-C(25)	115.6(19)

C(21)-N(3)-Pt(1)	125.1(15)
C(25)-N(3)-Pt(1)	119.2(15)
N(2A)-C(1A)-C(2A)	110.1(15)
N(2A)-C(1A)-Pt(2)	115.3(13)
C(2A)-C(1A)-Pt(2)	134.0(15)
N(2)-C(1)-C(2)	116(2)
N(2)-C(1)-Pt(1)	116.2(19)
C(2)-C(1)-Pt(1)	128(2)
C(3A)-C(2A)-C(1A)	105.2(17)
C(1)-C(2)-C(3)	94(2)
C(8)-C(3)-C(4)	124(2)
C(8)-C(3)-C(2)	116(2)
C(4)-C(3)-C(2)	121(2)
C(4A)-C(3A)-C(2A)	132(2)
C(4A)-C(3A)-C(8A)	115(2)
C(2A)-C(3A)-C(8A)	113.2(19)
C(3)-C(4)-C(5)	114(2)
C(3A)-C(4A)-C(5A)	112(2)
C(6A)-C(5A)-C(4A)	130(3)
C(6)-C(5)-C(4)	116(2)
C(5A)-C(6A)-C(7A)	118(3)
C(7)-C(6)-C(5)	125(3)
C(6A)-C(7A)-C(8A)	118(2)
C(6A)-C(7A)-C(9A)	119(2)
C(8A)-C(7A)-C(9A)	123(2)
C(6)-C(7)-C(8)	117(3)
C(6)-C(7)-C(9)	113(2)
C(8)-C(7)-C(9)	129(2)
C(3)-C(8)-C(7)	123(2)
C(3)-C(8)-N(2)	107(2)
C(7)-C(8)-N(2)	129(2)
C(7A)-C(8A)-C(3A)	126(2)
C(7A)-C(8A)-N(2A)	134(2)
C(3A)-C(8A)-N(2A)	99.3(17)
N(1A)-C(10A)-C(11A)	135(2)
N(1A)-C(10A)-N(2A)	108(2)

C(11A)-C(10A)-N(2A)	116(2)
N(1)-C(10)-N(2)	118(2)
N(1)-C(10)-C(11)	120(2)
N(2)-C(10)-C(11)	121(2)
C(12)-C(11)-C(10)	121(2)
C(12A)-C(11A)-C(10A)	112(2)
C(11A)-C(12A)-C(13A)	122(2)
C(11)-C(12)-C(13)	119(2)
C(12A)-C(13A)-C(14A)	114(2)
C(12A)-C(13A)-B(1A)	122(2)
C(14A)-C(13A)-B(1A)	123(2)
C(14)-C(13)-C(12)	108(2)
C(14)-C(13)-B(1)	135(2)
C(12)-C(13)-B(1)	116(2)
N(1A)-C(14A)-C(13A)	126.1(19)
N(1)-C(14)-C(13)	138(2)
C(16A)-C(15A)-C(20A)	112(2)
C(16A)-C(15A)-Pt(2)	130.9(17)
C(20A)-C(15A)-Pt(2)	117.2(15)
C(20)-C(15)-C(16)	112(2)
C(20)-C(15)-Pt(1)	126.0(17)
C(16)-C(15)-Pt(1)	122.1(18)
C(15)-C(16)-C(17)	122(3)
C(15A)-C(16A)-C(17A)	135(2)
C(18)-C(17)-C(16)	125(3)
C(18A)-C(17A)-C(16A)	116(2)
C(17A)-C(18A)-C(19A)	117(2)
C(17)-C(18)-C(19)	113(3)
C(18A)-C(19A)-C(20A)	123(3)
C(18)-C(19)-C(20)	118(3)
C(15)-C(20)-C(19)	129(3)
C(19A)-C(20A)-C(15A)	117(2)
N(3A)-C(21A)-C(22A)	123.6(17)
N(3)-C(21)-C(22)	119(2)
C(23)-C(22)-C(21)	124(2)
C(23A)-C(22A)-C(21A)	119(2)

C(22A)-C(23A)-C(24A)	119(2)
C(22A)-C(23A)-C(26A)	120(2)
C(24A)-C(23A)-C(26A)	120(2)
C(22)-C(23)-C(24)	123(3)
C(22)-C(23)-C(26)	120(3)
C(24)-C(23)-C(26)	117(3)
C(23A)-C(24A)-C(25A)	116(2)
C(23)-C(24)-C(25)	112(2)
N(3A)-C(25A)-C(24A)	131.1(19)
N(3)-C(25)-C(24)	126(2)
C(26)-C(26A)-C(23A)	121(2)
C(26A)-C(26)-C(23)	131(3)
C(28A)-C(27A)-C(32A)	120.0
C(28A)-C(27A)-B(1A)	120.1(18)
C(32A)-C(27A)-B(1A)	119.9(18)
C(27A)-C(28A)-C(29A)	120.0
C(27A)-C(28A)-C(33A)	119(2)
C(29A)-C(28A)-C(33A)	121(2)
C(28A)-C(29A)-C(30A)	120.0
C(29A)-C(30A)-C(31A)	120.0
C(29A)-C(30A)-C(34A)	126(2)
C(31A)-C(30A)-C(34A)	113(2)
C(32A)-C(31A)-C(30A)	120.0
C(31A)-C(32A)-C(27A)	120.0
C(31A)-C(32A)-C(35A)	118(2)
C(27A)-C(32A)-C(35A)	122(2)
C(28)-C(27)-C(32)	120.0
C(28)-C(27)-B(1)	126(2)
C(32)-C(27)-B(1)	114(2)
C(29)-C(28)-C(27)	120.0
C(29)-C(28)-C(35)	121(2)
C(27)-C(28)-C(35)	119(2)
C(30)-C(29)-C(28)	120.0
C(29)-C(30)-C(31)	120.0
C(29)-C(30)-C(34)	107(2)
C(31)-C(30)-C(34)	132(2)

C(32)-C(31)-C(30)	120.0
C(31)-C(32)-C(27)	120.0
C(31)-C(32)-C(33)	104(2)
C(27)-C(32)-C(33)	135(2)
C(37A)-C(36A)-C(41A)	120.0
C(37A)-C(36A)-B(1A)	124.8(16)
C(41A)-C(36A)-B(1A)	114.9(16)
C(38A)-C(37A)-C(36A)	120.0
C(38A)-C(37A)-C(42A)	122.2(18)
C(36A)-C(37A)-C(42A)	117.8(18)
C(37A)-C(38A)-C(39A)	120.0
C(40A)-C(39A)-C(38A)	120.0
C(40A)-C(39A)-C(43A)	125(2)
C(38A)-C(39A)-C(43A)	115(2)
C(39A)-C(40A)-C(41A)	120.0
C(40A)-C(41A)-C(36A)	120.0
C(40A)-C(41A)-C(44A)	111.0(17)
C(36A)-C(41A)-C(44A)	128.2(17)
C(37)-C(36)-C(41)	120.0
C(37)-C(36)-B(1)	120.9(18)
C(41)-C(36)-B(1)	119.1(18)
C(38)-C(37)-C(36)	120.0
C(38)-C(37)-C(44)	119.2(16)
C(36)-C(37)-C(44)	120.4(16)
C(37)-C(38)-C(39)	120.0
C(38)-C(39)-C(40)	120.0
C(38)-C(39)-C(43)	123(2)
C(40)-C(39)-C(43)	116(2)
C(41)-C(40)-C(39)	120.0
C(40)-C(41)-C(36)	120.0
C(40)-C(41)-C(42)	119.8(19)
C(36)-C(41)-C(42)	120.1(19)
C(13A)-B(1A)-C(27A)	117(2)
C(13A)-B(1A)-C(36A)	122(2)
C(27A)-B(1A)-C(36A)	120.8(18)
C(13)-B(1)-C(36)	125(2)

C(13)-B(1)-C(27)	116(2)
C(36)-B(1)-C(27)	119(2)

Table SD4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound4B'. 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)	46(1)	118(1)	60(1)	-21(1)	18(1)	22(1)
Pt(2)	47(1)	52(1)	64(1)	-7(1)	25(1)	9(1)
N(1)	19(9)	76(14)	42(11)	-7(9)	-1(8)	-20(9)
N(2A)	48(11)	69(13)	84(14)	29(11)	34(10)	28(10)
N(2)	46(11)	69(14)	60(12)	7(10)	11(9)	35(11)
N(3A)	20(9)	116(15)	57(12)	0(10)	17(8)	25(10)
C(2A)	49(12)	26(11)	39(12)	9(9)	22(10)	6(10)
C(2)	77(16)	86(18)	50(14)	-32(13)	8(13)	58(15)
C(4A)	40(13)	48(15)	130(20)	-21(16)	42(15)	-4(11)
C(5A)	110(20)	39(17)	110(30)	-10(17)	70(20)	-42(16)
C(5)	63(17)	67(19)	100(20)	-25(15)	45(17)	8(15)
C(6A)	71(17)	51(16)	62(17)	2(13)	25(13)	28(13)
C(6)	53(16)	80(20)	80(20)	-49(16)	31(15)	2(17)
C(7)	14(11)	120(20)	42(15)	-21(14)	8(11)	-4(13)
C(9A)	170(30)	140(20)	120(20)	100(20)	90(20)	100(20)
C(9)	66(17)	160(30)	29(14)	5(16)	-23(12)	40(17)
B(1A)	33(15)	90(20)	100(20)	14(17)	2(15)	45(15)

Table SD5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **4B**'.

	x	y	z	U(eq)
H(2AA)	-8399	-9552	-5143	45
H(2A)	-11692	-16393	-8701	84
H(4A)	-13990	-17252	-9160	111
H(4AA)	-9183	-9249	-3972	92
H(5AA)	-8933	-9567	-2863	116
H(5A)	-15765	-17442	-10053	93
H(6AA)	-7899	-10231	-2413	71
H(6A)	-15767	-16533	-10710	95
H(9AA)	-5839	-10561	-2974	170
H(9AB)	-6783	-11314	-2969	170
H(9AC)	-6333	-10600	-2362	170
H(9A)	-15097	-15719	-11225	140
H(9B)	-13789	-15407	-11085	140
H(9C)	-14375	-14925	-10725	140
H(11A)	-13367	-14250	-10041	104
H(11B)	-7519	-11896	-3883	94
H(12A)	-6888	-12923	-4154	118
H(12B)	-12683	-12974	-9967	99
H(14A)	-5988	-11916	-5617	75
H(14B)	-9732	-13192	-9229	64
H(16A)	-10006	-15506	-7733	132
H(16B)	-5663	-9304	-6250	73
H(17A)	-9058	-16195	-7122	151
H(17B)	-5897	-8437	-6888	86
H(18A)	-7680	-8336	-7268	95
H(18B)	-7938	-16787	-7520	148
H(19A)	-9123	-9213	-7045	152
H(19B)	-7451	-16358	-8466	141

H(20A)	-8424	-15663	-9044	123
H(20B)	-8760	-10040	-6269	105
H(21A)	-7358	-11107	-7103	50
H(21B)	-7855	-13844	-7669	87
H(22A)	-6173	-12873	-7500	92
H(22B)	-6546	-11451	-7902	71
H(24A)	-3801	-11178	-6405	72
H(24B)	-6752	-12894	-9432	106
H(25A)	-4641	-10771	-5691	54
H(25B)	-8529	-13822	-9598	102
H(26A)	-3875	-11322	-7715	116
H(26B)	-4778	-12342	-8557	137
H(29A)	-5932	-15320	-4127	175
H(31A)	-9000	-15259	-5000	215
H(29B)	-7029	-10281	-8432	246
H(31B)	-7505	-11827	-10071	230
H(33A)	-4415	-13947	-3871	177
H(33B)	-4540	-13541	-4498	177
H(33C)	-4374	-14356	-4564	177
H(33D)	-8859	-12361	-10720	146
H(33E)	-10041	-12303	-10730	146
H(33F)	-9648	-12958	-10427	146
H(34A)	-8003	-16175	-3957	238
H(34B)	-7945	-16565	-4651	238
H(34C)	-8963	-16278	-4632	238
H(34D)	-5574	-10485	-9378	204
H(34E)	-5476	-10975	-8808	204
H(34F)	-5632	-10163	-8662	204
H(35A)	-9197	-13940	-5360	244
H(35B)	-9021	-14334	-6014	244
H(35C)	-8226	-13496	-5629	244
H(35D)	-9815	-11028	-8360	202
H(35E)	-9203	-10188	-8438	202
H(35F)	-8594	-10562	-7880	202
H(38A)	-5202	-14070	-7108	162
H(40A)	-3041	-12161	-5809	172

H(38B)	-13009	-11060	-8656	89
H(40B)	-12178	-10205	-10190	192
H(42A)	-11403	-11049	-10893	245
H(42B)	-10601	-11434	-10465	245
H(42C)	-10264	-10528	-10351	245
H(42D)	-6861	-14690	-6073	253
H(42E)	-6796	-14897	-6811	253
H(42F)	-7398	-14303	-6647	253
H(43A)	-13810	-10021	-9772	346
H(43B)	-12660	-9449	-9276	346
H(43C)	-13528	-9985	-8986	346
H(43D)	-3545	-12847	-7396	338
H(43E)	-3345	-13610	-7209	338
H(43F)	-2505	-12799	-6786	338
H(44A)	-11708	-11697	-7994	150
H(44B)	-11114	-12130	-8395	150
H(44C)	-12420	-12467	-8531	150
H(44D)	-2942	-11942	-4725	169
H(44E)	-3929	-12344	-4451	169
H(44F)	-3977	-11645	-4813	169

Table SD6. Crystal data and structure refinement for compound **4A**.

Identification code	**4A**	
Empirical formula	C94 H96 B2 N6 Pt2	
Formula weight	1721.56	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.376(2) Å	α= 102.840(4)°.
	b = 15.757(3) Å	β= 91.661(4)°.
	c = 21.260(3) Å	γ = 99.232(4)°.
Volume	4302.7(12) $Å^3$	
Z	2	
Density (calculated)	1.329 Mg/m^3	
Absorption coefficient	3.294 mm^{-1}	
F(000)	1736	
Crystal size	0.160 x 0.040 x 0.024 mm^3	
Theta range for data collection	2.217 to 27.214°.	
Index ranges	-17<=h<=17, -20<=k<=20, -26<=l<=27	
Reflections collected	71702	
Independent reflections	18868 [R(int) = 0.2129]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.925 and 0.621	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18868 / 0 / 950	
Goodness-of-fit on F^2	0.867	
Final R indices [I>2sigma(I)]	R1 = 0.0725, wR2 = 0.1255	
R indices (all data)	R1 = 0.1981, wR2 = 0.1566	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.383 and -1.157 $e.Å^{-3}$	

Table SD7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4A**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4157(1)	883(1)	897(1)	37(1)
Pt(2)	8690(1)	4926(1)	4297(1)	56(1)
N(1)	4922(5)	1750(5)	369(4)	34(2)
N(2)	3309(5)	1544(5)	-106(4)	34(2)
N(3)	5452(6)	711(5)	1403(4)	40(2)
N(4)	7728(6)	4724(8)	5022(5)	61(3)
N(5)	8147(7)	6257(9)	5326(5)	78(3)
N(6)	8637(6)	3604(6)	3853(4)	53(3)
B(1)	5948(11)	2953(13)	5626(7)	73(5)
B(2)	7464(8)	3331(7)	344(5)	36(3)
C(1)	3022(7)	1020(6)	368(4)	29(2)
C(2)	1977(7)	787(6)	269(4)	37(2)
C(3)	1609(6)	1101(6)	-234(5)	35(2)
C(4)	619(7)	1041(7)	-531(5)	46(3)
C(5)	511(8)	1462(8)	-1009(5)	58(3)
C(6)	1340(7)	1937(8)	-1248(5)	60(3)
C(7)	2316(7)	2019(7)	-969(5)	49(3)
C(8)	2448(6)	1613(6)	-463(4)	30(2)
C(9)	4325(7)	1949(6)	-78(5)	39(3)
C(10)	4701(7)	2514(6)	-466(5)	45(3)
C(11)	5703(7)	2941(7)	-345(5)	47(3)
C(12)	6332(6)	2781(6)	132(5)	35(2)
C(13)	5895(6)	2182(6)	478(5)	35(2)
C(14)	3285(7)	142(7)	1411(5)	42(3)
C(15)	2467(7)	447(7)	1716(5)	43(3)
C(16)	1862(8)	-23(8)	2079(5)	54(3)
C(17)	2052(9)	-839(9)	2133(6)	67(4)

C(18)	2832(9)	-1145(8)	1844(6)	63(3)
C(19)	3439(7)	-678(7)	1477(5)	47(3)
C(20)	1364(11)	-1371(12)	2542(10)	155(9)
C(21)	507(10)	-1090(10)	2813(7)	101(5)
C(22)	-104(12)	-1603(12)	3240(9)	131(7)
C(23)	-1015(17)	-1303(14)	3473(10)	189(10)
C(24)	5550(7)	847(7)	2054(5)	44(3)
C(25)	6378(8)	771(7)	2372(6)	53(3)
C(26)	7222(7)	500(7)	2048(6)	49(3)
C(27)	8154(8)	391(9)	2388(7)	70(4)
C(28)	8712(8)	943(9)	2890(6)	68(4)
C(29)	7106(7)	314(6)	1373(6)	47(3)
C(30)	6224(7)	430(6)	1068(5)	44(3)
C(31)	8622(8)	1845(8)	3224(6)	54(3)
C(32)	9041(8)	2180(10)	3844(6)	65(4)
C(33)	9011(8)	3036(10)	4141(6)	66(4)
C(34)	8272(7)	3262(8)	3221(5)	44(3)
C(35)	8248(7)	2419(8)	2909(6)	51(3)
C(36)	8181(7)	3012(7)	775(5)	43(3)
C(37)	8444(7)	2169(8)	583(5)	45(3)
C(38)	9143(8)	1932(8)	985(6)	61(3)
C(39)	9616(8)	2473(11)	1523(7)	66(4)
C(40)	9349(10)	3291(10)	1720(6)	70(4)
C(41)	8635(8)	3577(9)	1352(6)	58(3)
C(42)	8385(9)	4488(8)	1600(5)	72(4)
C(43)	8033(8)	1528(7)	-55(5)	58(3)
C(44)	10403(10)	2181(11)	1915(7)	111(6)
C(45)	7741(7)	4186(6)	79(5)	40(3)
C(46)	7186(7)	4890(7)	224(5)	47(3)
C(47)	7485(8)	5658(7)	-4(5)	54(3)
C(48)	8313(8)	5753(7)	-358(5)	47(3)
C(49)	8836(7)	5074(6)	-515(5)	43(3)
C(50)	8582(7)	4297(7)	-304(5)	41(3)
C(51)	9167(7)	3547(6)	-532(5)	52(3)
C(52)	6291(8)	4889(7)	655(5)	65(4)
C(53)	8607(9)	6596(7)	-601(6)	76(4)

C(54)	8690(8)	6158(10)	4742(5)	63(4)
C(55)	9029(10)	6988(11)	4656(7)	80(4)
C(56)	8695(11)	7637(13)	5186(9)	93(6)
C(57)	8790(12)	8580(13)	5392(10)	121(7)
C(58)	8348(18)	8887(19)	5983(14)	189(17)
C(59)	7900(20)	8450(20)	6332(15)	197(16)
C(60)	7772(13)	7553(14)	6185(9)	129(7)
C(61)	8177(12)	7160(12)	5601(8)	96(5)
C(62)	7610(10)	5480(11)	5454(6)	67(4)
C(63)	6974(9)	5486(11)	5951(6)	80(4)
C(64)	6485(9)	4704(11)	6005(6)	73(4)
C(65)	6546(8)	3876(10)	5594(7)	70(4)
C(66)	7213(8)	3981(9)	5094(5)	64(4)
C(67)	9614(7)	5250(8)	3655(5)	55(3)
C(68)	10497(8)	4844(8)	3507(5)	60(3)
C(69)	11168(8)	5093(9)	3059(6)	68(4)
C(70)	11011(9)	5685(9)	2718(6)	68(4)
C(71)	10157(8)	6058(8)	2812(5)	64(4)
C(72)	9484(8)	5847(7)	3271(5)	56(3)
C(73)	11730(10)	5980(11)	2255(7)	99(5)
C(74)	12684(9)	5739(11)	2220(7)	103(5)
C(75)	13414(9)	6121(10)	1765(6)	86(5)
C(76)	14280(10)	5721(11)	1657(7)	112(6)
C(77)	5022(10)	2917(11)	6108(7)	98(5)
C(78)	4230(10)	3405(11)	6058(7)	91(5)
C(79)	3499(10)	3509(13)	6545(8)	126(7)
C(80)	3534(11)	3078(13)	7027(8)	114(6)
C(81)	4274(12)	2551(13)	7068(7)	115(6)
C(82)	5036(13)	2461(12)	6610(7)	111(6)
C(83)	5849(12)	1862(12)	6656(9)	140(8)
C(84)	2801(11)	3187(15)	7557(8)	178(10)
C(85)	4093(9)	3820(12)	5492(7)	123(7)
C(86)	6249(11)	2108(11)	5247(7)	84(5)
C(87)	5514(17)	1492(17)	4811(10)	134(8)
C(88)	5769(18)	727(18)	4454(12)	151(10)
C(89)	6670(30)	570(15)	4475(14)	174(14)

C(90)	7488(15)	1151(15)	4939(11)	115(6)
C(91)	7228(12)	1922(12)	5281(8)	92(5)
C(92)	8061(9)	2521(10)	5768(7)	101(5)
C(93)	4417(13)	1582(14)	4704(9)	178(10)
C(94)	7043(17)	-274(17)	4102(11)	200(9)

Table SD8. Bond lengths [Å] and angles [°] for **4A**.

Pt(1)-C(1)	1.933(9)
Pt(1)-C(14)	2.028(9)
Pt(1)-N(3)	2.098(8)
Pt(1)-N(1)	2.116(7)
Pt(2)-C(54)	1.960(15)
Pt(2)-C(67)	1.963(11)
Pt(2)-N(6)	2.077(10)
Pt(2)-N(4)	2.082(9)
N(1)-C(9)	1.345(11)
N(1)-C(13)	1.356(10)
N(2)-C(8)	1.393(11)
N(2)-C(9)	1.400(10)
N(2)-C(1)	1.460(10)
N(3)-C(24)	1.350(12)
N(3)-C(30)	1.350(12)
N(4)-C(66)	1.302(13)
N(4)-C(62)	1.368(15)
N(5)-C(62)	1.403(16)
N(5)-C(61)	1.408(17)
N(5)-C(54)	1.449(14)
N(6)-C(33)	1.339(13)
N(6)-C(34)	1.374(12)
B(1)-C(86)	1.52(2)
B(1)-C(65)	1.56(2)
B(1)-C(77)	1.631(18)
B(2)-C(36)	1.523(15)
B(2)-C(45)	1.569(14)

B(2)-C(12)	1.616(13)
C(1)-C(2)	1.384(11)
C(2)-C(3)	1.383(11)
C(3)-C(4)	1.429(12)
C(3)-C(8)	1.437(11)
C(4)-C(5)	1.348(13)
C(5)-C(6)	1.408(13)
C(6)-C(7)	1.393(13)
C(7)-C(8)	1.388(12)
C(9)-C(10)	1.389(12)
C(10)-C(11)	1.390(12)
C(11)-C(12)	1.390(13)
C(12)-C(13)	1.389(11)
C(14)-C(19)	1.378(13)
C(14)-C(15)	1.386(13)
C(15)-C(16)	1.377(12)
C(16)-C(17)	1.377(15)
C(17)-C(18)	1.329(15)
C(17)-C(20)	1.559(15)
C(18)-C(19)	1.381(13)
C(20)-C(21)	1.390(18)
C(21)-C(22)	1.518(15)
C(22)-C(23)	1.44(2)
C(24)-C(25)	1.316(13)
C(25)-C(26)	1.415(14)
C(26)-C(29)	1.399(14)
C(26)-C(27)	1.477(14)
C(27)-C(28)	1.336(16)
C(28)-C(31)	1.467(16)
C(29)-C(30)	1.386(13)
C(31)-C(32)	1.372(15)
C(31)-C(35)	1.383(14)
C(32)-C(33)	1.363(16)
C(34)-C(35)	1.341(14)
C(36)-C(41)	1.401(14)
C(36)-C(37)	1.404(14)

C(37)-C(38)	1.397(14)
C(37)-C(43)	1.526(14)
C(38)-C(39)	1.338(16)
C(39)-C(40)	1.371(16)
C(39)-C(44)	1.513(16)
C(40)-C(41)	1.408(16)
C(41)-C(42)	1.508(15)
C(45)-C(46)	1.416(13)
C(45)-C(50)	1.418(12)
C(46)-C(47)	1.405(13)
C(46)-C(52)	1.529(12)
C(47)-C(48)	1.365(13)
C(48)-C(49)	1.357(13)
C(48)-C(53)	1.527(13)
C(49)-C(50)	1.391(12)
C(50)-C(51)	1.519(13)
C(54)-C(55)	1.368(17)
C(55)-C(56)	1.47(2)
C(56)-C(61)	1.41(2)
C(56)-C(57)	1.44(2)
C(57)-C(58)	1.42(3)
C(58)-C(59)	1.23(4)
C(59)-C(60)	1.36(3)
C(60)-C(61)	1.42(2)
C(62)-C(63)	1.375(16)
C(63)-C(64)	1.330(16)
C(64)-C(65)	1.416(17)
C(65)-C(66)	1.427(15)
C(67)-C(72)	1.403(14)
C(67)-C(68)	1.441(15)
C(68)-C(69)	1.402(14)
C(69)-C(70)	1.339(15)
C(70)-C(71)	1.366(16)
C(70)-C(73)	1.491(15)
C(71)-C(72)	1.403(14)
C(73)-C(74)	1.388(16)

C(74)-C(75)	1.542(14)
C(75)-C(76)	1.407(16)
C(77)-C(82)	1.415(18)
C(77)-C(78)	1.419(18)
C(78)-C(79)	1.446(18)
C(78)-C(85)	1.512(16)
C(79)-C(80)	1.353(18)
C(80)-C(81)	1.40(2)
C(80)-C(84)	1.514(19)
C(81)-C(82)	1.432(19)
C(82)-C(83)	1.56(2)
C(86)-C(91)	1.391(19)
C(86)-C(87)	1.42(2)
C(87)-C(88)	1.37(3)
C(87)-C(93)	1.51(3)
C(88)-C(89)	1.28(4)
C(89)-C(90)	1.49(3)
C(89)-C(94)	1.55(3)
C(90)-C(91)	1.37(2)
C(91)-C(92)	1.538(19)

C(1)-Pt(1)-C(14)	94.2(4)
C(1)-Pt(1)-N(3)	175.3(4)
C(14)-Pt(1)-N(3)	89.1(3)
C(1)-Pt(1)-N(1)	80.4(3)
C(14)-Pt(1)-N(1)	173.0(4)
N(3)-Pt(1)-N(1)	96.6(3)
C(54)-Pt(2)-C(67)	93.6(5)
C(54)-Pt(2)-N(6)	177.3(4)
C(67)-Pt(2)-N(6)	89.1(4)
C(54)-Pt(2)-N(4)	80.5(5)
C(67)-Pt(2)-N(4)	174.0(5)
N(6)-Pt(2)-N(4)	96.9(4)
C(9)-N(1)-C(13)	117.9(7)
C(9)-N(1)-Pt(1)	114.3(5)
C(13)-N(1)-Pt(1)	127.4(6)

C(8)-N(2)-C(9)	132.1(7)
C(8)-N(2)-C(1)	110.1(6)
C(9)-N(2)-C(1)	117.5(7)
C(24)-N(3)-C(30)	117.4(8)
C(24)-N(3)-Pt(1)	123.5(7)
C(30)-N(3)-Pt(1)	119.1(7)
C(66)-N(4)-C(62)	117.5(11)
C(66)-N(4)-Pt(2)	128.0(9)
C(62)-N(4)-Pt(2)	114.4(8)
C(62)-N(5)-C(61)	133.4(14)
C(62)-N(5)-C(54)	116.4(12)
C(61)-N(5)-C(54)	109.6(13)
C(33)-N(6)-C(34)	115.0(10)
C(33)-N(6)-Pt(2)	123.1(9)
C(34)-N(6)-Pt(2)	121.8(7)
C(86)-B(1)-C(65)	121.0(12)
C(86)-B(1)-C(77)	120.6(14)
C(65)-B(1)-C(77)	118.3(14)
C(36)-B(2)-C(45)	124.3(9)
C(36)-B(2)-C(12)	120.3(8)
C(45)-B(2)-C(12)	115.4(9)
C(2)-C(1)-N(2)	104.4(8)
C(2)-C(1)-Pt(1)	141.8(7)
N(2)-C(1)-Pt(1)	113.8(6)
C(3)-C(2)-C(1)	111.6(8)
C(2)-C(3)-C(4)	134.0(8)
C(2)-C(3)-C(8)	108.0(8)
C(4)-C(3)-C(8)	117.9(8)
C(5)-C(4)-C(3)	119.2(9)
C(4)-C(5)-C(6)	122.7(10)
C(7)-C(6)-C(5)	120.0(10)
C(8)-C(7)-C(6)	118.6(9)
C(7)-C(8)-N(2)	132.4(8)
C(7)-C(8)-C(3)	121.6(8)
N(2)-C(8)-C(3)	105.9(7)
N(1)-C(9)-C(10)	122.0(8)

N(1)-C(9)-N(2)	113.7(8)
C(10)-C(9)-N(2)	124.3(9)
C(9)-C(10)-C(11)	118.4(9)
C(10)-C(11)-C(12)	121.1(9)
C(13)-C(12)-C(11)	116.1(8)
C(13)-C(12)-B(2)	120.3(9)
C(11)-C(12)-B(2)	123.2(8)
N(1)-C(13)-C(12)	124.2(9)
C(19)-C(14)-C(15)	115.6(9)
C(19)-C(14)-Pt(1)	124.1(8)
C(15)-C(14)-Pt(1)	120.3(8)
C(16)-C(15)-C(14)	122.6(10)
C(15)-C(16)-C(17)	119.5(10)
C(18)-C(17)-C(16)	119.0(10)
C(18)-C(17)-C(20)	121.5(12)
C(16)-C(17)-C(20)	119.4(12)
C(17)-C(18)-C(19)	121.7(11)
C(14)-C(19)-C(18)	121.6(10)
C(21)-C(20)-C(17)	122.4(13)
C(20)-C(21)-C(22)	120.5(14)
C(23)-C(22)-C(21)	117.4(15)
C(25)-C(24)-N(3)	123.4(10)
C(24)-C(25)-C(26)	121.7(11)
C(29)-C(26)-C(25)	115.2(9)
C(29)-C(26)-C(27)	121.5(11)
C(25)-C(26)-C(27)	123.2(11)
C(28)-C(27)-C(26)	129.1(12)
C(27)-C(28)-C(31)	130.3(11)
C(30)-C(29)-C(26)	120.1(10)
N(3)-C(30)-C(29)	121.9(10)
C(32)-C(31)-C(35)	117.7(12)
C(32)-C(31)-C(28)	119.6(12)
C(35)-C(31)-C(28)	122.1(12)
C(33)-C(32)-C(31)	119.6(12)
N(6)-C(33)-C(32)	124.0(11)
C(35)-C(34)-N(6)	123.9(10)

C(34)-C(35)-C(31)	119.6(11)
C(41)-C(36)-C(37)	119.0(10)
C(41)-C(36)-B(2)	120.2(10)
C(37)-C(36)-B(2)	120.7(10)
C(38)-C(37)-C(36)	117.8(11)
C(38)-C(37)-C(43)	119.4(11)
C(36)-C(37)-C(43)	122.7(10)
C(39)-C(38)-C(37)	124.1(12)
C(38)-C(39)-C(40)	118.2(12)
C(38)-C(39)-C(44)	120.9(15)
C(40)-C(39)-C(44)	120.9(14)
C(39)-C(40)-C(41)	121.4(12)
C(36)-C(41)-C(40)	119.3(12)
C(36)-C(41)-C(42)	122.6(11)
C(40)-C(41)-C(42)	118.1(12)
C(46)-C(45)-C(50)	116.9(9)
C(46)-C(45)-B(2)	121.9(8)
C(50)-C(45)-B(2)	121.2(9)
C(47)-C(46)-C(45)	119.9(9)
C(47)-C(46)-C(52)	116.7(9)
C(45)-C(46)-C(52)	123.2(9)
C(48)-C(47)-C(46)	121.6(10)
C(49)-C(48)-C(47)	119.0(9)
C(49)-C(48)-C(53)	120.9(10)
C(47)-C(48)-C(53)	120.0(11)
C(48)-C(49)-C(50)	122.1(9)
C(49)-C(50)-C(45)	120.3(9)
C(49)-C(50)-C(51)	118.9(9)
C(45)-C(50)-C(51)	120.6(9)
C(55)-C(54)-N(5)	107.1(13)
C(55)-C(54)-Pt(2)	138.8(11)
N(5)-C(54)-Pt(2)	114.0(10)
C(54)-C(55)-C(56)	108.7(14)
C(61)-C(56)-C(57)	114.7(19)
C(61)-C(56)-C(55)	107.3(15)
C(57)-C(56)-C(55)	137.9(18)

C(58)-C(57)-C(56)	115(2)
C(59)-C(58)-C(57)	128(3)
C(58)-C(59)-C(60)	121(3)
C(59)-C(60)-C(61)	116(2)
N(5)-C(61)-C(56)	107.2(16)
N(5)-C(61)-C(60)	128(2)
C(56)-C(61)-C(60)	124.5(19)
N(4)-C(62)-C(63)	123.1(14)
N(4)-C(62)-N(5)	114.3(11)
C(63)-C(62)-N(5)	122.5(15)
C(64)-C(63)-C(62)	116.3(15)
C(63)-C(64)-C(65)	126.1(13)
C(64)-C(65)-C(66)	110.8(11)
C(64)-C(65)-B(1)	127.3(13)
C(66)-C(65)-B(1)	121.8(14)
N(4)-C(66)-C(65)	126.1(13)
C(72)-C(67)-C(68)	112.3(10)
C(72)-C(67)-Pt(2)	125.7(9)
C(68)-C(67)-Pt(2)	121.9(9)
C(69)-C(68)-C(67)	121.7(11)
C(70)-C(69)-C(68)	122.8(12)
C(69)-C(70)-C(71)	118.2(11)
C(69)-C(70)-C(73)	123.7(13)
C(71)-C(70)-C(73)	118.0(12)
C(70)-C(71)-C(72)	120.6(11)
C(67)-C(72)-C(71)	124.2(11)
C(74)-C(73)-C(70)	120.6(12)
C(73)-C(74)-C(75)	117.7(12)
C(76)-C(75)-C(74)	114.3(12)
C(82)-C(77)-C(78)	119.1(13)
C(82)-C(77)-B(1)	120.8(14)
C(78)-C(77)-B(1)	119.9(12)
C(77)-C(78)-C(79)	121.0(12)
C(77)-C(78)-C(85)	122.2(13)
C(79)-C(78)-C(85)	116.8(13)
C(80)-C(79)-C(78)	118.8(16)

C(79)-C(80)-C(81)	121.3(14)
C(79)-C(80)-C(84)	120.6(17)
C(81)-C(80)-C(84)	118.0(15)
C(80)-C(81)-C(82)	121.5(15)
C(77)-C(82)-C(81)	118.1(17)
C(77)-C(82)-C(83)	120.9(15)
C(81)-C(82)-C(83)	121.0(14)
C(91)-C(86)-C(87)	117.8(18)
C(91)-C(86)-B(1)	123.3(15)
C(87)-C(86)-B(1)	118.8(17)
C(88)-C(87)-C(86)	120(2)
C(88)-C(87)-C(93)	114(2)
C(86)-C(87)-C(93)	125(2)
C(89)-C(88)-C(87)	122(3)
C(88)-C(89)-C(90)	122(2)
C(88)-C(89)-C(94)	126(3)
C(90)-C(89)-C(94)	111(3)
C(91)-C(90)-C(89)	115(2)
C(90)-C(91)-C(86)	122.7(17)
C(90)-C(91)-C(92)	115.3(17)
C(86)-C(91)-C(92)	121.7(17)

Symmetry transformations used to generate equivalent atoms:

Table SD9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4A**. 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)	28(1)	34(1)	50(1)	12(1)	5(1)	3(1)
Pt(2)	38(1)	83(1)	46(1)	16(1)	-1(1)	7(1)
N(1)	21(4)	30(5)	50(6)	2(4)	12(4)	8(4)
N(2)	19(4)	37(5)	52(5)	21(4)	8(4)	7(4)
N(3)	35(5)	28(5)	61(6)	15(4)	8(4)	5(4)
N(4)	33(5)	78(8)	69(7)	12(7)	-4(5)	9(5)
N(5)	47(6)	115(11)	62(8)	1(8)	-25(6)	14(7)
N(6)	37(5)	84(7)	52(7)	44(6)	9(4)	16(5)
B(1)	57(10)	117(15)	46(10)	16(10)	0(7)	22(10)
B(2)	46(7)	18(6)	35(7)	-14(5)	21(6)	6(5)
C(1)	32(5)	20(5)	37(6)	4(4)	6(4)	11(4)
C(2)	38(6)	34(6)	35(6)	5(5)	-4(5)	2(5)
C(3)	27(5)	47(7)	41(6)	31(5)	9(4)	6(5)
C(4)	18(5)	50(7)	69(8)	15(6)	3(5)	5(5)
C(5)	30(6)	82(9)	63(8)	15(7)	2(5)	14(6)
C(6)	28(6)	88(9)	68(8)	26(7)	5(5)	5(6)
C(7)	31(6)	55(7)	58(8)	11(6)	7(5)	3(5)
C(8)	24(5)	29(6)	39(6)	8(5)	9(4)	7(4)
C(9)	23(5)	38(6)	59(7)	14(6)	9(5)	6(5)
C(10)	30(6)	55(7)	64(8)	36(6)	15(5)	14(5)
C(11)	29(6)	49(7)	68(8)	25(6)	11(5)	4(5)
C(12)	17(5)	38(6)	55(7)	17(5)	17(5)	6(4)
C(13)	22(5)	45(6)	45(7)	15(5)	2(4)	17(5)
C(14)	37(6)	46(7)	38(6)	10(5)	-3(5)	-6(5)
C(15)	38(6)	47(7)	45(7)	9(6)	4(5)	7(5)
C(16)	49(7)	68(9)	49(8)	17(7)	12(6)	16(6)
C(17)	57(8)	75(10)	88(10)	60(8)	9(7)	2(7)

C(18)	54(8)	56(8)	87(10)	31(7)	7(7)	10(6)
C(19)	38(6)	41(7)	58(8)	12(6)	-6(5)	0(5)
C(20)	77(11)	199(19)	270(20)	198(19)	94(14)	64(12)
C(21)	81(11)	132(14)	84(11)	45(10)	4(8)	-28(10)
C(22)	118(14)	148(16)	172(18)	112(14)	78(13)	36(12)
C(23)	240(30)	190(20)	160(20)	78(16)	136(19)	51(19)
C(24)	30(6)	59(8)	45(7)	12(6)	8(5)	7(5)
C(25)	47(7)	56(8)	63(8)	10(6)	-10(6)	40(6)
C(26)	33(6)	39(7)	78(9)	27(6)	-1(6)	1(5)
C(27)	49(8)	74(10)	101(11)	34(8)	0(7)	32(7)
C(28)	31(6)	91(11)	92(11)	42(9)	-14(6)	14(7)
C(29)	36(6)	39(7)	69(9)	13(6)	-8(5)	11(5)
C(30)	39(6)	39(7)	52(7)	15(5)	3(5)	-3(5)
C(31)	42(7)	54(8)	68(9)	19(7)	1(6)	10(6)
C(32)	37(7)	89(11)	72(10)	25(8)	-18(6)	18(7)
C(33)	44(7)	103(12)	51(8)	25(8)	-16(6)	7(7)
C(34)	39(6)	59(8)	42(7)	20(6)	2(5)	19(6)
C(35)	39(6)	65(9)	53(8)	25(7)	9(5)	10(6)
C(36)	22(5)	48(7)	59(8)	14(6)	7(5)	2(5)
C(37)	19(5)	61(8)	58(8)	24(7)	6(5)	0(5)
C(38)	34(7)	65(9)	94(11)	39(8)	18(7)	9(6)
C(39)	24(6)	92(11)	89(11)	40(9)	-9(6)	5(7)
C(40)	63(9)	100(12)	42(8)	23(8)	16(7)	-7(8)
C(41)	37(7)	90(11)	50(8)	26(8)	11(6)	2(7)
C(42)	84(9)	65(9)	41(8)	-28(6)	-10(6)	-8(7)
C(43)	50(7)	41(7)	83(9)	8(7)	16(6)	17(6)
C(44)	78(10)	155(15)	125(14)	82(12)	2(9)	21(10)
C(45)	26(5)	31(6)	58(7)	-1(5)	5(5)	1(5)
C(46)	35(6)	35(7)	69(8)	7(6)	18(5)	2(5)
C(47)	46(7)	47(7)	73(8)	11(6)	21(6)	20(6)
C(48)	47(7)	30(7)	58(8)	8(6)	3(6)	-7(5)
C(49)	29(6)	36(7)	59(7)	-2(6)	18(5)	1(5)
C(50)	28(5)	42(7)	52(7)	10(6)	2(5)	2(5)
C(51)	48(7)	40(7)	62(8)	0(6)	19(6)	8(5)
C(52)	50(7)	69(9)	87(10)	30(7)	31(7)	17(6)
C(53)	76(9)	46(8)	113(12)	33(8)	25(8)	4(7)

C(54)	48(7)	104(12)	38(8)	14(8)	0(6)	19(7)
C(55)	75(10)	82(11)	67(10)	-12(9)	-19(8)	16(9)
C(56)	62(10)	106(15)	113(15)	56(14)	-50(9)	-15(10)
C(57)	104(13)	85(14)	170(20)	42(13)	-84(13)	-7(11)
C(58)	120(20)	190(30)	170(30)	-160(20)	-73(18)	80(20)
C(59)	140(20)	250(40)	130(30)	-60(20)	6(17)	-20(20)
C(60)	126(15)	113(16)	97(15)	-52(13)	-47(11)	-9(13)
C(61)	103(12)	90(13)	64(11)	-43(11)	-60(9)	23(10)
C(62)	61(9)	110(13)	32(8)	17(8)	-7(6)	22(9)
C(63)	57(9)	132(14)	55(9)	27(9)	-3(7)	19(9)
C(64)	55(8)	119(13)	41(8)	6(9)	-2(6)	22(9)
C(65)	39(7)	99(12)	74(10)	33(9)	-10(7)	-1(7)
C(66)	46(7)	100(11)	41(8)	14(7)	-1(6)	6(7)
C(67)	21(6)	73(9)	60(8)	5(7)	-5(5)	-6(6)
C(68)	40(7)	91(10)	47(8)	20(7)	-6(5)	0(6)
C(69)	29(6)	110(11)	65(9)	14(8)	8(6)	16(7)
C(70)	43(8)	109(12)	52(8)	30(8)	-12(6)	-6(7)
C(71)	39(7)	87(10)	60(8)	31(7)	-19(6)	-20(7)
C(72)	42(7)	60(8)	62(8)	14(7)	-5(6)	-7(6)
C(73)	63(9)	165(15)	78(11)	51(10)	5(8)	11(10)
C(74)	50(8)	187(17)	93(11)	67(11)	12(7)	29(10)
C(75)	44(8)	139(13)	86(10)	53(9)	28(7)	8(8)
C(76)	66(10)	167(17)	128(14)	62(12)	30(9)	48(10)
C(77)	61(9)	193(17)	66(10)	68(11)	13(7)	38(10)
C(78)	50(8)	154(14)	90(11)	74(11)	-5(7)	21(9)
C(79)	56(9)	250(20)	99(13)	86(14)	26(9)	21(11)
C(80)	47(9)	200(19)	117(15)	85(14)	27(9)	13(10)
C(81)	71(11)	220(20)	70(11)	60(12)	27(9)	18(12)
C(82)	107(13)	149(16)	74(12)	49(11)	-14(10)	-18(12)
C(83)	88(12)	210(20)	168(18)	129(16)	15(11)	41(13)
C(84)	77(12)	370(30)	108(15)	105(18)	38(10)	21(15)
C(85)	54(9)	230(20)	112(13)	106(14)	0(8)	31(10)
C(86)	49(9)	113(13)	85(11)	28(10)	3(8)	-7(9)
C(87)	131(19)	160(20)	92(15)	12(14)	41(14)	-13(17)
C(88)	130(20)	170(30)	140(20)	4(17)	55(17)	-5(18)
C(89)	270(40)	78(16)	170(20)	12(15)	150(30)	10(20)

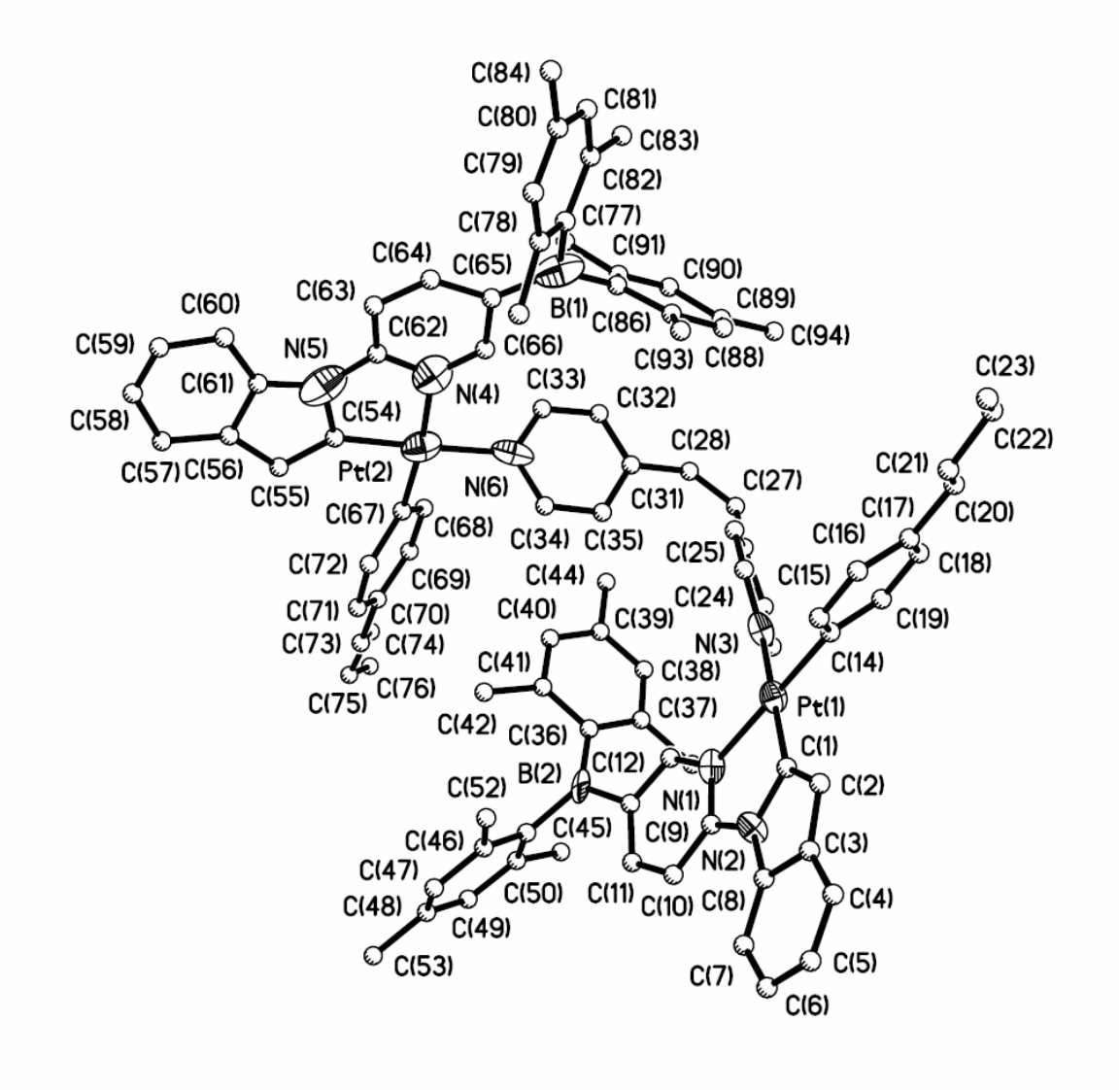
C(90)	123(16)	98(15)	153(19)	74(14)	48(14)	37(14)
C(91)	84(12)	86(13)	122(14)	54(11)	33(10)	16(10)
C(92)	45(8)	146(15)	125(14)	61(12)	-1(8)	14(9)
C(93)	67(12)	260(30)	180(20)	38(18)	-18(12)	-32(14)
C(94)	204	210(30)	190(20)	70(20)	56(19)	10(20)

Table SD10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4A**.

	x	y	z	U(eq)
H(2A)	1564	453	515	44
H(4A)	45	708	-393	55
H(5A)	-152	1438	-1192	70
H(6A)	1234	2201	-1599	72
H(7A)	2880	2345	-1122	58
H(10A)	4283	2605	-805	54
H(11A)	5963	3350	-593	57
H(13A)	6304	2068	812	42
H(15A)	2318	1002	1674	52
H(16A)	1318	213	2291	64
H(18A)	2976	-1700	1891	76
H(19A)	3976	-928	1266	56
H(20A)	1137	-1970	2265	186
H(20B)	1808	-1441	2902	186
H(21A)	38	-1060	2452	121
H(21B)	721	-478	3070	121
H(22A)	-292	-2225	2996	158
H(22B)	345	-1598	3620	158
H(23A)	-1506	-1808	3533	284
H(23B)	-1308	-1027	3158	284
H(23C)	-853	-871	3887	284
H(24A)	4994	1005	2294	53
H(25A)	6409	902	2831	63
H(27A)	8391	-149	2227	85
H(28A)	9252	716	3057	81
H(29A)	7632	107	1122	57
H(30A)	6162	308	609	52
H(32A)	9349	1817	4066	78

H(33A)	9273	3243	4578	79
H(34A)	8022	3646	2992	53
H(35A)	7977	2218	2474	61
H(38A)	9292	1350	868	73
H(40A)	9651	3671	2113	83
H(42A)	7656	4441	1661	108
H(42B)	8566	4849	1287	108
H(42C)	8769	4764	2014	108
H(43A)	8584	1248	-258	86
H(43B)	7757	1851	-344	86
H(43C)	7496	1073	28	86
H(44A)	10276	1535	1838	167
H(44B)	10360	2438	2376	167
H(44C)	11081	2381	1786	167
H(47A)	7100	6123	91	65
H(49A)	9395	5131	-778	52
H(51A)	9392	3339	-160	77
H(51B)	9759	3758	-751	77
H(51C)	8726	3061	-834	77
H(52A)	6491	4749	1062	98
H(52B)	5718	4443	433	98
H(52C)	6089	5473	745	98
H(53A)	9298	6626	-746	114
H(53B)	8578	7111	-250	114
H(53C)	8134	6591	-963	114
H(55A)	9415	7125	4313	96
H(57A)	9123	8970	5152	145
H(58A)	8409	9510	6125	226
H(59A)	7631	8743	6713	236
H(60A)	7434	7210	6455	154
H(63A)	6889	6020	6240	96
H(64A)	6054	4700	6353	88
H(66A)	7289	3461	4786	77
H(68A)	10628	4398	3717	72
H(69A)	11759	4830	2994	82
H(71A)	10018	6464	2565	77

H(72A)	8904	6126	3324	68
H(73A)	11383	5767	1818	119
H(73B)	11832	6633	2354	119
H(74A)	12589	5087	2085	124
H(74B)	13021	5913	2661	124
H(75A)	13040	6056	1343	103
H(75B)	13635	6761	1950	103
H(76A)	14749	6050	1415	168
H(76B)	14078	5110	1408	168
H(76C)	14616	5722	2073	168
H(79A)	3004	3874	6527	152
H(81A)	4269	2247	7407	138
H(83A)	5729	1587	7024	210
H(83B)	6529	2222	6716	210
H(83C)	5800	1401	6256	210
H(84A)	2789	2707	7783	267
H(84B)	2119	3167	7366	267
H(84C)	3020	3756	7864	267
H(85A)	4627	3704	5194	184
H(85B)	4135	4459	5649	184
H(85C)	3427	3566	5265	184
H(88A)	5258	304	4184	181
H(90A)	8139	1000	4994	138
H(92A)	8724	2500	5585	152
H(92B)	8060	2315	6170	152
H(92C)	7931	3129	5858	152
H(93A)	4042	1026	4439	266
H(93B)	4382	2060	4482	266
H(93C)	4117	1717	5122	266
H(94A)	6836	-381	3642	300
H(94B)	6741	-780	4271	300
H(94C)	7784	-194	4159	300



A crystal structure diagram of **4A** with labeling schemes.

Table SD11. Crystal data and structure refinement for **4B**.

Identification code	**4B**	
Empirical formula	C104 H116 B2 Cl16 N6 Pt2	
Formula weight	2429.02	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.180(5) Å	α= 92.37°.
	b = 14.222(6) Å	β= 93.759(9)°.
	c = 14.222(6) Å	γ = 93.759(9)°.
Volume	2853(2) $Å^3$	
Z	1	
Density (calculated)	1.414 Mg/m^3	
Absorption coefficient	2.869 mm^{-1}	
F(000)	1220	
Crystal size	0.240 x 0.240 x 0.230 mm^3	
Theta range for data collection	2.874 to 28.485°.	
Index ranges	-19<=h<=17, -19<=k<=19, -18<=l<=19	
Reflections collected	62881	
Independent reflections	14194 [R(int) = 0.0701]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.558 and 0.546	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14194 / 0 / 597	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1147	
R indices (all data)	R1 = 0.0696, wR2 = 0.1220	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.507 and -1.674 $e.Å^{-3}$	

Table SD12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4B**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1199(1)	6092(1)	594(1)	25(1)
B(1)	3096(4)	2856(4)	1549(4)	30(1)
N(1)	1959(3)	4908(3)	327(2)	28(1)
N(2)	2004(3)	5557(3)	-1120(2)	26(1)
N(3)	792(3)	5690(3)	1921(3)	28(1)
C(1)	1617(3)	6364(3)	-670(3)	26(1)
C(2)	1659(3)	7067(3)	-1291(3)	29(1)
C(3)	2037(4)	6725(3)	-2161(3)	32(1)
C(4)	2179(4)	7141(4)	-3011(3)	40(1)
C(5)	2447(4)	6590(4)	-3759(4)	47(1)
C(6)	2507(4)	5631(4)	-3675(3)	44(1)
C(7)	2365(3)	5176(4)	-2837(3)	34(1)
C(8)	2209(3)	5771(3)	-2059(3)	30(1)
C(9)	2265(5)	4111(4)	-2877(4)	49(1)
C(10)	2320(3)	4880(3)	-543(3)	26(1)
C(11)	3010(3)	4258(3)	-740(3)	33(1)
C(12)	3265(4)	3617(3)	-95(3)	32(1)
C(13)	2837(3)	3590(3)	779(3)	30(1)
C(14)	2207(3)	4269(3)	955(3)	28(1)
C(16)	281(3)	4867(3)	2011(3)	31(1)
C(17)	15(4)	4560(4)	2865(3)	36(1)
C(18)	242(4)	5109(4)	3681(3)	36(1)
C(19)	769(4)	5974(4)	3586(3)	40(1)
C(20)	1026(4)	6229(3)	2697(3)	35(1)
C(21)	504(3)	7262(3)	785(3)	26(1)
C(22)	917(4)	8183(3)	736(3)	34(1)
C(23)	400(4)	8976(3)	910(4)	39(1)

C(24)	-527(4)	8874(4)	1115(3)	38(1)
C(25)	-949(4)	7971(4)	1171(4)	40(1)
C(26)	-435(4)	7189(3)	1016(3)	34(1)
C(27)	-1094(5)	9724(4)	1292(4)	56(2)
C(28)	-934(6)	10195(5)	2262(5)	63(2)
C(29)	-1269(7)	9614(6)	3031(5)	86(3)
C(30)	-1142(10)	10113(7)	3993(7)	131(5)
C(31)	3991(3)	2292(3)	1402(3)	32(1)
C(32)	4906(4)	2761(4)	1387(4)	39(1)
C(33)	5691(4)	2252(4)	1246(4)	47(1)
C(34)	5609(4)	1272(5)	1106(5)	56(2)
C(35)	4700(4)	820(4)	1106(4)	48(1)
C(36)	3901(4)	1303(4)	1254(4)	37(1)
C(37)	2948(4)	755(4)	1228(5)	51(2)
C(38)	6492(5)	739(6)	969(6)	79(2)
C(39)	5096(4)	3819(4)	1546(5)	53(2)
C(40)	2450(4)	2737(3)	2415(3)	32(1)
C(41)	1473(4)	2472(3)	2300(3)	34(1)
C(42)	926(4)	2370(4)	3083(4)	41(1)
C(43)	1323(5)	2541(4)	3997(4)	47(1)
C(44)	2279(5)	2804(4)	4119(4)	52(2)
C(45)	2851(4)	2900(4)	3357(4)	45(1)
C(46)	3908(5)	3200(6)	3562(5)	84(3)
C(47)	970(4)	2239(4)	1338(4)	43(1)
C(48)	726(6)	2415(5)	4849(4)	67(2)
C(49)	3632(5)	7224(5)	1018(5)	74(2)
C(50)	4288(8)	6209(9)	4190(9)	138(4)
C(51)	-89(4)	4783(4)	4592(4)	42(1)
C(52)	5849(12)	8390(20)	2808(12)	323(17)
C(53)	1416(12)	-1066(8)	3389(9)	192(8)
Cl(1)	4216(2)	6192(2)	1203(2)	84(1)
Cl(2)	3430(2)	7866(2)	2037(2)	115(1)
Cl(3)	5298(2)	5647(2)	3830(2)	95(1)
Cl(4)	3250(2)	5676(3)	3770(2)	148(1)
Cl(5)	1718(4)	149(2)	3448(3)	183(2)
Cl(6)	2017(3)	-1681(2)	4113(2)	154(2)

Cl(7)	6167(3)	8230(3)	1775(3)	180(2)
Cl(8)	6466(4)	8215(3)	3787(4)	221(2)

Table SD13. Bond lengths [Å] and angles [°] for **4B**

Pt(1)-C(1)	1.976(4)
Pt(1)-C(21)	2.007(5)
Pt(1)-N(1)	2.092(4)
Pt(1)-N(3)	2.099(4)
B(1)-C(31)	1.566(7)
B(1)-C(13)	1.585(7)
B(1)-C(40)	1.591(7)
N(1)-C(14)	1.347(6)
N(1)-C(10)	1.370(5)
N(2)-C(10)	1.369(6)
N(2)-C(8)	1.427(5)
N(2)-C(1)	1.447(6)
N(3)-C(20)	1.329(6)
N(3)-C(16)	1.350(6)
C(1)-C(2)	1.362(6)
C(2)-C(3)	1.459(6)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.389(7)
C(3)-C(8)	1.405(7)
C(4)-C(5)	1.384(8)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.382(8)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(7)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.403(7)
C(7)-C(9)	1.510(8)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.396(6)
C(11)-C(12)	1.368(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.419(6)

C(12)-H(12A)	0.9500
C(13)-C(14)	1.384(7)
C(14)-H(14A)	0.9500
C(16)-C(17)	1.376(6)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.380(7)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.413(7)
C(18)-C(51)	1.487(7)
C(19)-C(20)	1.395(6)
C(19)-H(19A)	0.9500
C(20)-H(20A)	0.9500
C(21)-C(26)	1.392(6)
C(21)-C(22)	1.406(6)
C(22)-C(23)	1.408(7)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.364(8)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.388(7)
C(24)-C(27)	1.517(7)
C(25)-C(26)	1.387(7)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-C(28)	1.504(8)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.482(10)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.510(11)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(36)	1.409(7)

C(31)-C(32)	1.423(7)
C(32)-C(33)	1.388(8)
C(32)-C(39)	1.515(8)
C(33)-C(34)	1.396(9)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.402(9)
C(34)-C(38)	1.525(9)
C(35)-C(36)	1.386(7)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.513(8)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(41)	1.409(7)
C(40)-C(45)	1.425(7)
C(41)-C(42)	1.405(7)
C(41)-C(47)	1.514(7)
C(42)-C(43)	1.388(8)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.381(9)
C(43)-C(48)	1.533(7)
C(44)-C(45)	1.400(8)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.537(9)
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800

C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-Cl(2)	1.731(8)
C(49)-Cl(1)	1.754(8)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-Cl(4)	1.672(11)
C(50)-Cl(3)	1.780(11)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-C(51)#1	1.294(11)
C(51)-H(51A)	0.93(6)
C(52)-Cl(7)	1.577(17)
C(52)-Cl(8)	1.631(18)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-Cl(6)	1.615(10)
C(53)-Cl(5)	1.750(13)
C(53)-H(54A)	0.9900
C(53)-H(54B)	0.9900

C(1)-Pt(1)-C(21)	96.86(17)
C(1)-Pt(1)-N(1)	79.82(16)
C(21)-Pt(1)-N(1)	176.59(14)
C(1)-Pt(1)-N(3)	175.30(16)
C(21)-Pt(1)-N(3)	87.75(15)
N(1)-Pt(1)-N(3)	95.59(14)
C(31)-B(1)-C(13)	116.9(4)
C(31)-B(1)-C(40)	124.0(4)
C(13)-B(1)-C(40)	119.1(4)
C(14)-N(1)-C(10)	119.3(4)
C(14)-N(1)-Pt(1)	126.2(3)
C(10)-N(1)-Pt(1)	113.9(3)
C(10)-N(2)-C(8)	131.3(4)
C(10)-N(2)-C(1)	116.9(3)

C(8)-N(2)-C(1)	109.2(4)
C(20)-N(3)-C(16)	117.8(4)
C(20)-N(3)-Pt(1)	121.6(3)
C(16)-N(3)-Pt(1)	120.6(3)
C(2)-C(1)-N(2)	106.6(4)
C(2)-C(1)-Pt(1)	141.3(4)
N(2)-C(1)-Pt(1)	112.1(3)
C(1)-C(2)-C(3)	109.8(4)
C(1)-C(2)-H(2A)	125.1
C(3)-C(2)-H(2A)	125.1
C(4)-C(3)-C(8)	120.0(5)
C(4)-C(3)-C(2)	132.4(5)
C(8)-C(3)-C(2)	107.5(4)
C(5)-C(4)-C(3)	118.8(5)
C(5)-C(4)-H(4A)	120.6
C(3)-C(4)-H(4A)	120.6
C(6)-C(5)-C(4)	120.1(5)
C(6)-C(5)-H(5A)	119.9
C(4)-C(5)-H(5A)	119.9
C(5)-C(6)-C(7)	123.2(5)
C(5)-C(6)-H(6A)	118.4
C(7)-C(6)-H(6A)	118.4
C(6)-C(7)-C(8)	115.2(5)
C(6)-C(7)-C(9)	118.2(5)
C(8)-C(7)-C(9)	126.0(4)
C(7)-C(8)-C(3)	121.6(4)
C(7)-C(8)-N(2)	130.6(4)
C(3)-C(8)-N(2)	106.6(4)
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(2)-C(10)-N(1)	113.7(4)
N(2)-C(10)-C(11)	126.0(4)

N(1)-C(10)-C(11)	120.1(4)
C(12)-C(11)-C(10)	119.9(4)
C(12)-C(11)-H(11A)	120.0
C(10)-C(11)-H(11A)	120.0
C(11)-C(12)-C(13)	120.2(4)
C(11)-C(12)-H(12A)	119.9
C(13)-C(12)-H(12A)	119.9
C(14)-C(13)-C(12)	116.8(4)
C(14)-C(13)-B(1)	120.8(4)
C(12)-C(13)-B(1)	122.4(4)
N(1)-C(14)-C(13)	123.3(4)
N(1)-C(14)-H(14A)	118.3
C(13)-C(14)-H(14A)	118.3
N(3)-C(16)-C(17)	123.0(5)
N(3)-C(16)-H(16A)	118.5
C(17)-C(16)-H(16A)	118.5
C(16)-C(17)-C(18)	120.4(5)
C(16)-C(17)-H(17A)	119.8
C(18)-C(17)-H(17A)	119.8
C(17)-C(18)-C(19)	116.5(4)
C(17)-C(18)-C(51)	119.6(5)
C(19)-C(18)-C(51)	123.9(5)
C(20)-C(19)-C(18)	119.7(5)
C(20)-C(19)-H(19A)	120.2
C(18)-C(19)-H(19A)	120.2
N(3)-C(20)-C(19)	122.6(4)
N(3)-C(20)-H(20A)	118.7
C(19)-C(20)-H(20A)	118.7
C(26)-C(21)-C(22)	116.0(4)
C(26)-C(21)-Pt(1)	119.8(3)
C(22)-C(21)-Pt(1)	124.1(3)
C(21)-C(22)-C(23)	121.2(5)
C(21)-C(22)-H(22A)	119.4
C(23)-C(22)-H(22A)	119.4
C(24)-C(23)-C(22)	121.0(5)
C(24)-C(23)-H(23A)	119.5

C(22)-C(23)-H(23A)	119.5
C(23)-C(24)-C(25)	118.8(5)
C(23)-C(24)-C(27)	121.3(5)
C(25)-C(24)-C(27)	119.9(5)
C(26)-C(25)-C(24)	120.4(5)
C(26)-C(25)-H(25A)	119.8
C(24)-C(25)-H(25A)	119.8
C(25)-C(26)-C(21)	122.6(5)
C(25)-C(26)-H(26A)	118.7
C(21)-C(26)-H(26A)	118.7
C(28)-C(27)-C(24)	115.6(5)
C(28)-C(27)-H(27A)	108.4
C(24)-C(27)-H(27A)	108.4
C(28)-C(27)-H(27B)	108.4
C(24)-C(27)-H(27B)	108.4
H(27A)-C(27)-H(27B)	107.5
C(29)-C(28)-C(27)	114.5(6)
C(29)-C(28)-H(28A)	108.6
C(27)-C(28)-H(28A)	108.6
C(29)-C(28)-H(28B)	108.6
C(27)-C(28)-H(28B)	108.6
H(28A)-C(28)-H(28B)	107.6
C(28)-C(29)-C(30)	113.8(8)
C(28)-C(29)-H(29A)	108.8
C(30)-C(29)-H(29A)	108.8
C(28)-C(29)-H(29B)	108.8
C(30)-C(29)-H(29B)	108.8
H(29A)-C(29)-H(29B)	107.7
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(36)-C(31)-C(32)	118.4(5)
C(36)-C(31)-B(1)	120.4(4)

C(32)-C(31)-B(1)	121.2(4)
C(33)-C(32)-C(31)	120.5(5)
C(33)-C(32)-C(39)	116.2(5)
C(31)-C(32)-C(39)	123.3(5)
C(32)-C(33)-C(34)	121.5(6)
C(32)-C(33)-H(33A)	119.3
C(34)-C(33)-H(33A)	119.3
C(35)-C(34)-C(33)	117.4(6)
C(35)-C(34)-C(38)	122.9(6)
C(33)-C(34)-C(38)	119.7(6)
C(36)-C(35)-C(34)	122.8(6)
C(36)-C(35)-H(35A)	118.6
C(34)-C(35)-H(35A)	118.6
C(35)-C(36)-C(31)	119.4(5)
C(35)-C(36)-C(37)	118.9(5)
C(31)-C(36)-C(37)	121.6(5)
C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(34)-C(38)-H(38A)	109.5
C(34)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(34)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(32)-C(39)-H(39A)	109.5
C(32)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(32)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(45)	116.9(5)
C(41)-C(40)-B(1)	122.8(4)

C(45)-C(40)-B(1)	120.3(5)
C(42)-C(41)-C(40)	121.2(5)
C(42)-C(41)-C(47)	116.7(5)
C(40)-C(41)-C(47)	122.1(4)
C(43)-C(42)-C(41)	121.3(5)
C(43)-C(42)-H(42A)	119.3
C(41)-C(42)-H(42A)	119.3
C(44)-C(43)-C(42)	118.1(5)
C(44)-C(43)-C(48)	120.8(6)
C(42)-C(43)-C(48)	121.1(6)
C(43)-C(44)-C(45)	122.3(5)
C(43)-C(44)-H(44A)	118.8
C(45)-C(44)-H(44A)	118.8
C(44)-C(45)-C(40)	120.2(5)
C(44)-C(45)-C(46)	118.6(5)
C(40)-C(45)-C(46)	121.2(5)
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(41)-C(47)-H(47A)	109.5
C(41)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(41)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(43)-C(48)-H(48A)	109.5
C(43)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(43)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
Cl(2)-C(49)-Cl(1)	114.7(5)
Cl(2)-C(49)-H(49A)	108.6

Cl(1)-C(49)-H(49A)	108.6
Cl(2)-C(49)-H(49B)	108.6
Cl(1)-C(49)-H(49B)	108.6
H(49A)-C(49)-H(49B)	107.6
Cl(4)-C(50)-Cl(3)	114.5(7)
Cl(4)-C(50)-H(50A)	108.6
Cl(3)-C(50)-H(50A)	108.6
Cl(4)-C(50)-H(50B)	108.6
Cl(3)-C(50)-H(50B)	108.6
H(50A)-C(50)-H(50B)	107.6
C(51)#1-C(51)-C(18)	125.9(7)
C(51)#1-C(51)-H(51A)	113(4)
C(18)-C(51)-H(51A)	121(4)
Cl(7)-C(52)-Cl(8)	126.6(12)
Cl(7)-C(52)-H(52A)	105.7
Cl(8)-C(52)-H(52A)	105.7
Cl(7)-C(52)-H(52B)	105.7
Cl(8)-C(52)-H(52B)	105.7
H(52A)-C(52)-H(52B)	106.1
Cl(6)-C(53)-Cl(5)	115.9(8)
Cl(6)-C(53)-H(54A)	108.3
Cl(5)-C(53)-H(54A)	108.3
Cl(6)-C(53)-H(54B)	108.3
Cl(5)-C(53)-H(54B)	108.3
H(54A)-C(53)-H(54B)	107.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table SD14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4B**. 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)	25(1)	31(1)	21(1)	3(1)	5(1)	4(1)
B(1)	28(3)	32(3)	29(3)	0(2)	-2(2)	1(2)
N(1)	29(2)	32(2)	23(2)	0(2)	5(2)	0(2)
N(2)	26(2)	35(2)	19(2)	2(2)	6(2)	6(2)
N(3)	27(2)	32(2)	26(2)	4(2)	3(2)	6(2)
C(1)	20(2)	33(2)	25(2)	2(2)	-2(2)	1(2)
C(2)	28(2)	32(2)	27(2)	5(2)	0(2)	2(2)
C(3)	30(3)	37(3)	28(2)	4(2)	2(2)	-2(2)
C(4)	43(3)	48(3)	30(3)	13(2)	7(2)	1(2)
C(5)	48(3)	67(4)	28(3)	15(3)	9(2)	3(3)
C(6)	40(3)	67(4)	26(2)	2(2)	9(2)	9(3)
C(7)	26(3)	48(3)	29(2)	3(2)	3(2)	5(2)
C(8)	25(2)	42(3)	23(2)	4(2)	2(2)	-2(2)
C(9)	61(4)	52(3)	35(3)	-5(2)	8(3)	13(3)
C(10)	25(2)	30(2)	22(2)	3(2)	4(2)	-1(2)
C(11)	33(3)	39(3)	29(2)	0(2)	11(2)	5(2)
C(12)	31(3)	37(3)	30(2)	2(2)	6(2)	10(2)
C(13)	24(2)	35(2)	31(2)	-1(2)	3(2)	2(2)
C(14)	29(2)	31(2)	25(2)	5(2)	3(2)	2(2)
C(16)	29(3)	34(2)	32(2)	6(2)	6(2)	5(2)
C(17)	32(3)	40(3)	38(3)	10(2)	5(2)	7(2)
C(18)	35(3)	44(3)	33(3)	12(2)	6(2)	11(2)
C(19)	48(3)	46(3)	24(2)	-4(2)	8(2)	0(3)
C(20)	47(3)	35(3)	23(2)	3(2)	5(2)	-1(2)
C(21)	25(2)	38(2)	15(2)	6(2)	2(2)	2(2)
C(22)	34(3)	36(3)	32(2)	4(2)	7(2)	5(2)

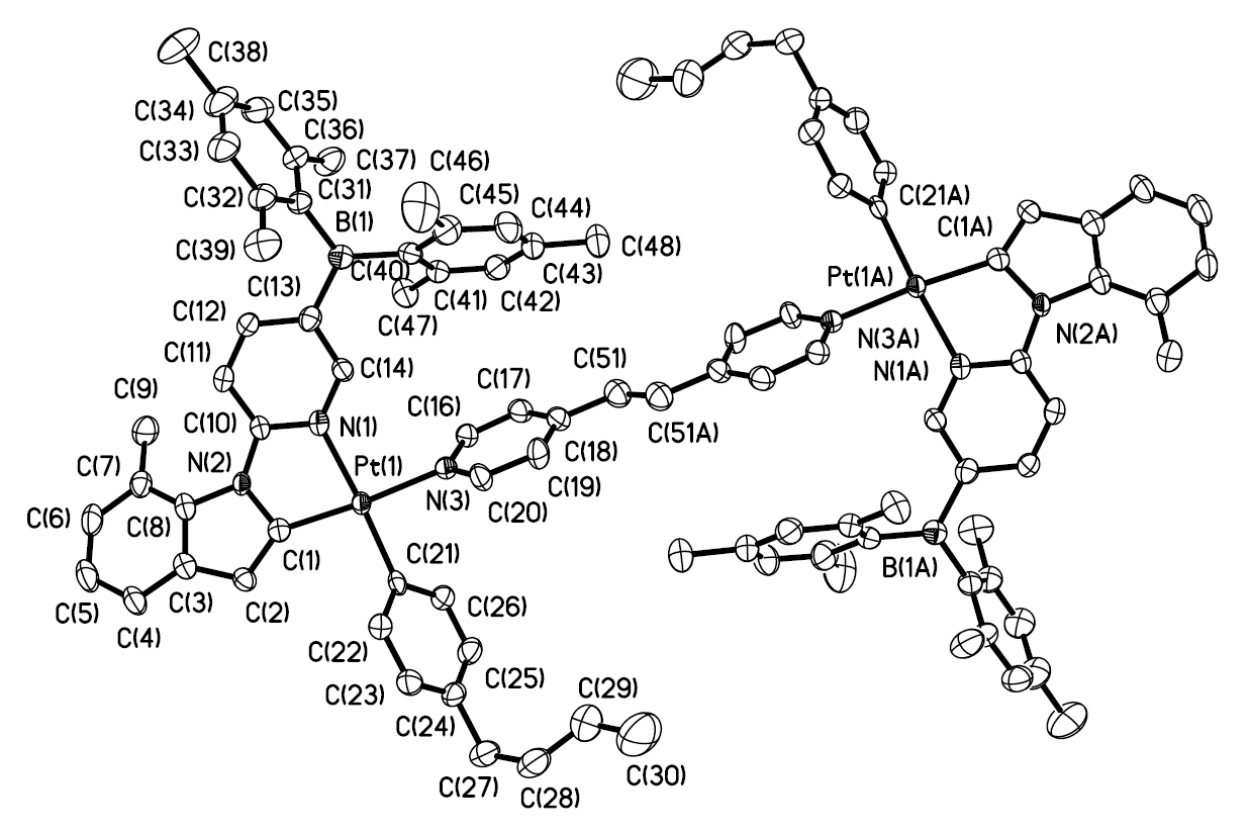
C(23)	52(3)	30(2)	36(3)	2(2)	9(2)	3(2)
C(24)	50(3)	42(3)	25(2)	1(2)	3(2)	20(3)
C(25)	33(3)	51(3)	39(3)	3(2)	7(2)	13(2)
C(26)	31(3)	37(3)	33(2)	3(2)	5(2)	6(2)
C(27)	76(5)	50(3)	48(3)	5(3)	11(3)	30(3)
C(28)	83(5)	54(4)	56(4)	-4(3)	10(4)	31(4)
C(29)	127(8)	76(5)	62(5)	2(4)	30(5)	31(5)
C(30)	206(14)	110(8)	81(7)	-21(6)	12(8)	65(9)
C(31)	26(2)	40(3)	31(2)	4(2)	0(2)	8(2)
C(32)	30(3)	46(3)	39(3)	1(2)	-1(2)	6(2)
C(33)	28(3)	61(4)	52(3)	1(3)	-6(2)	8(3)
C(34)	37(3)	74(4)	59(4)	-2(3)	-4(3)	22(3)
C(35)	50(4)	45(3)	50(3)	3(3)	-1(3)	15(3)
C(36)	35(3)	39(3)	40(3)	4(2)	5(2)	12(2)
C(37)	49(4)	36(3)	70(4)	-3(3)	12(3)	5(3)
C(38)	44(4)	90(5)	104(6)	-8(5)	0(4)	29(4)
C(39)	35(3)	49(3)	73(4)	2(3)	-3(3)	-4(3)
C(40)	39(3)	30(2)	30(2)	5(2)	2(2)	8(2)
C(41)	39(3)	30(2)	33(2)	4(2)	6(2)	7(2)
C(42)	41(3)	35(3)	49(3)	6(2)	12(2)	4(2)
C(43)	67(4)	41(3)	38(3)	8(2)	21(3)	16(3)
C(44)	72(5)	56(4)	28(3)	-1(2)	0(3)	10(3)
C(45)	48(3)	53(3)	34(3)	-6(2)	-6(2)	10(3)
C(46)	62(5)	137(7)	48(4)	-20(4)	-16(3)	-10(5)
C(47)	32(3)	57(3)	38(3)	7(2)	-1(2)	-3(3)
C(48)	97(6)	64(4)	47(4)	12(3)	35(4)	21(4)
C(49)	54(4)	89(5)	76(5)	7(4)	-6(4)	-5(4)
C(50)	84(8)	163(11)	167(12)	-20(9)	10(8)	10(8)
C(51)	42(3)	43(3)	41(3)	6(2)	5(2)	1(3)
C(52)	123(14)	690(50)	146(15)	-100(20)	-40(12)	80(20)
C(53)	296(19)	129(9)	145(11)	-59(8)	-121(11)	142(11)
Cl(1)	74(1)	71(1)	107(2)	0(1)	6(1)	4(1)
Cl(2)	97(2)	118(2)	127(2)	-31(2)	-9(2)	29(2)
Cl(3)	64(1)	120(2)	100(2)	-9(1)	14(1)	-3(1)
Cl(4)	84(2)	286(4)	81(2)	24(2)	12(1)	52(2)
Cl(5)	325(6)	105(2)	138(3)	44(2)	98(3)	56(3)

Cl(6)	273(5)	83(2)	102(2)	2(1)	-6(2)	5(2)
Cl(7)	156(3)	166(3)	209(4)	-75(3)	64(3)	-52(3)
Cl(8)	259(6)	185(4)	210(5)	59(4)	-34(4)	-30(4)

Table SD15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4B.

	x	y	z	U(eq)
H(2A)	1470	7688	-1174	35
H(4A)	2095	7793	-3078	48
H(5A)	2591	6871	-4332	57
H(6A)	2651	5262	-4212	53
H(9A)	1865	3895	-2381	73
H(9B)	2892	3865	-2782	73
H(9C)	1972	3882	-3495	73
H(11A)	3302	4279	-1322	40
H(12A)	3729	3189	-232	39
H(14A)	1937	4286	1549	34
H(16A)	97	4483	1458	38
H(17A)	-327	3965	2894	44
H(19A)	947	6379	4125	48
H(20A)	1383	6811	2644	42
H(22A)	1558	8272	582	40
H(23A)	700	9591	885	47
H(25A)	-1593	7889	1316	48
H(26A)	-737	6579	1070	40
H(27A)	-940	10197	824	68
H(27B)	-1776	9524	1182	68
H(28A)	-248	10363	2389	76
H(28B)	-1262	10789	2269	76
H(29A)	-919	9034	3045	104
H(29B)	-1948	9421	2891	104
H(30A)	-1477	9738	4446	196
H(30B)	-1401	10734	3963	196
H(30C)	-466	10190	4195	196
H(33A)	6298	2578	1245	57

H(35A)	4629	155	999	58
H(37A)	3041	79	1249	77
H(37B)	2577	876	645	77
H(37C)	2608	954	1772	77
H(38A)	6642	387	1531	118
H(38B)	7026	1189	868	118
H(38C)	6377	299	419	118
H(39A)	5572	3952	2074	80
H(39B)	4507	4101	1694	80
H(39C)	5329	4087	975	80
H(42A)	270	2180	2985	49
H(44A)	2560	2924	4741	62
H(46A)	4105	3055	4210	127
H(46B)	4012	3880	3484	127
H(46C)	4280	2857	3122	127
H(47A)	576	1648	1356	64
H(47B)	1439	2169	869	64
H(47C)	568	2749	1168	64
H(48A)	790	2996	5250	100
H(48B)	946	1892	5212	100
H(48C)	59	2278	4629	100
H(49A)	4013	7633	617	89
H(49B)	3015	7052	665	89
H(50A)	4307	6238	4887	166
H(50B)	4325	6865	3981	166
H(52A)	5248	7994	2832	387
H(52B)	5680	9051	2858	387
H(54A)	737	-1168	3507	231
H(54B)	1492	-1312	2739	231
H(51A)	-480(40)	4230(40)	4620(40)	50



A diagram showing the crystal structure of 4B with labeling schemes.