Electronic Supplementary Material (ESI) for Chemical Communications

Enhibiting olefin *cis, trans*-photoisomerization and enhancing electron-accepting ability of conjugated organoboron by metal chelation

Chul Baik and Suning Wang*

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

S1. Experimental Section

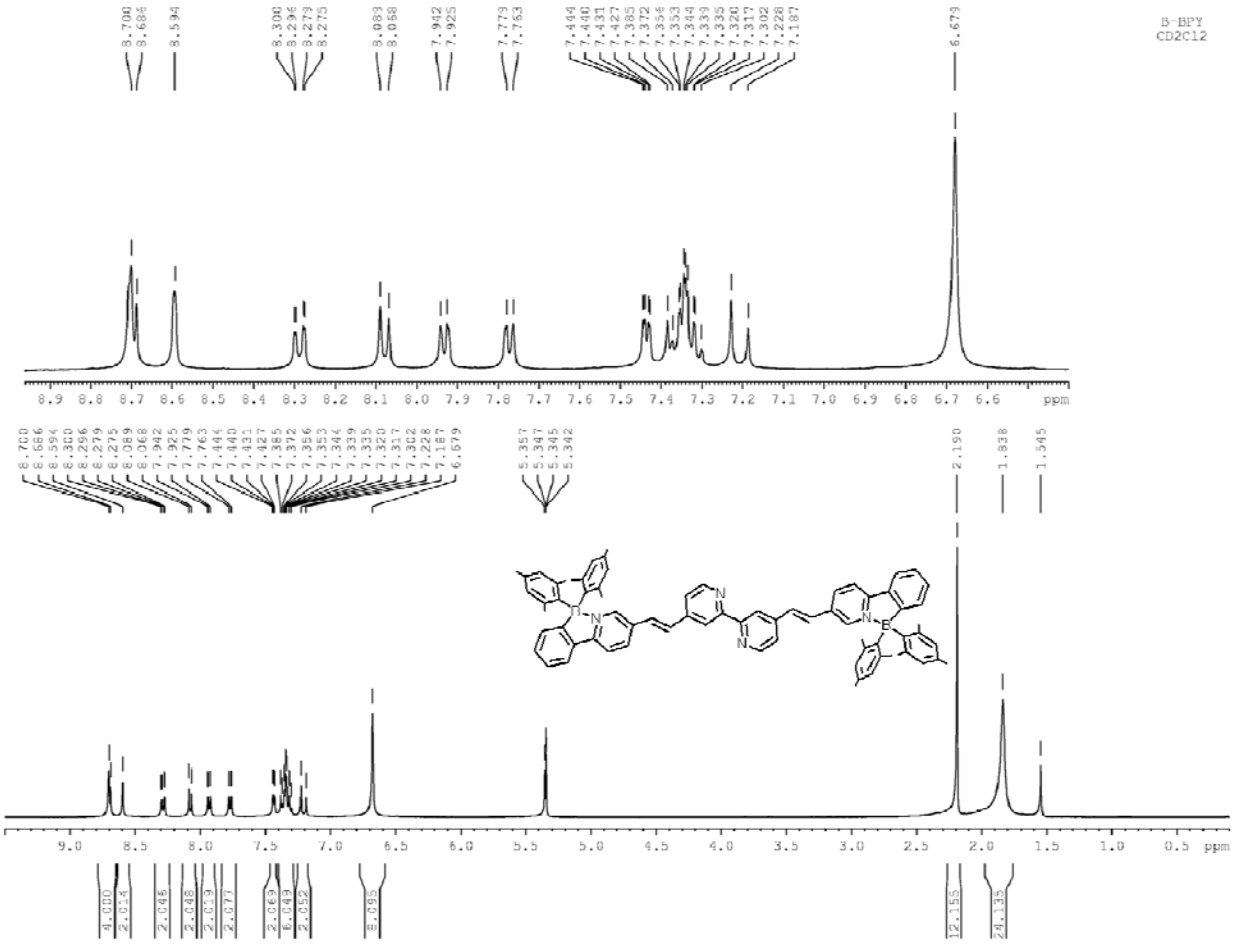
General Procedure. All experiments were performed under a nitrogen atmosphere in a Vacuum Atmospheres drybox or by standard Schlenk technique unless otherwise noted. THF, ether, and DMF were purified using the solvent purification system (Innovation Technology, Inc.). The ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded on Bruker Avance 300, 400 or 500 MHz spectrometers. UV-Vis spectra were recorded on an Ocean Optics UV-Visible spectrometer. Excitation and emission spectra were recorded on a Photon Technologies International Quanta Master model C-60 spectrometer. High resolution mass spectra (HRMS) were obtained from a Waters/Micromass GC-TOF EI-MS spectrometer which was internally calibrated before use. Elemental analyses were performed at the Canadian Microanalytical Service Ltd.. Cyclic voltammetry was performed using a BAS CV-50W analyzer with a scan rate of 200 mV/s and a typical concentration of 3 mg of the compounds in 3.0 mL of DMF. The electrolytic cell used was a conventional three-compartment cell, in which a Pt working electrode, a Pt auxiliary electrode, and a Ag/AgCl reference electrode were employed. **1**[1] and compound **2**[2] were prepared by modified methods describe in the reterature.

DFT Calculations on compounds : The Gaussian suit of programs (Gaussian 03) was used employing density functional theory (DFT). Calculations were performed at the B3LYP level of theory[3] using 6–31G*[4] as the basis set for all atoms except platinum and copper atoms, for which LAN2LDZ was used.

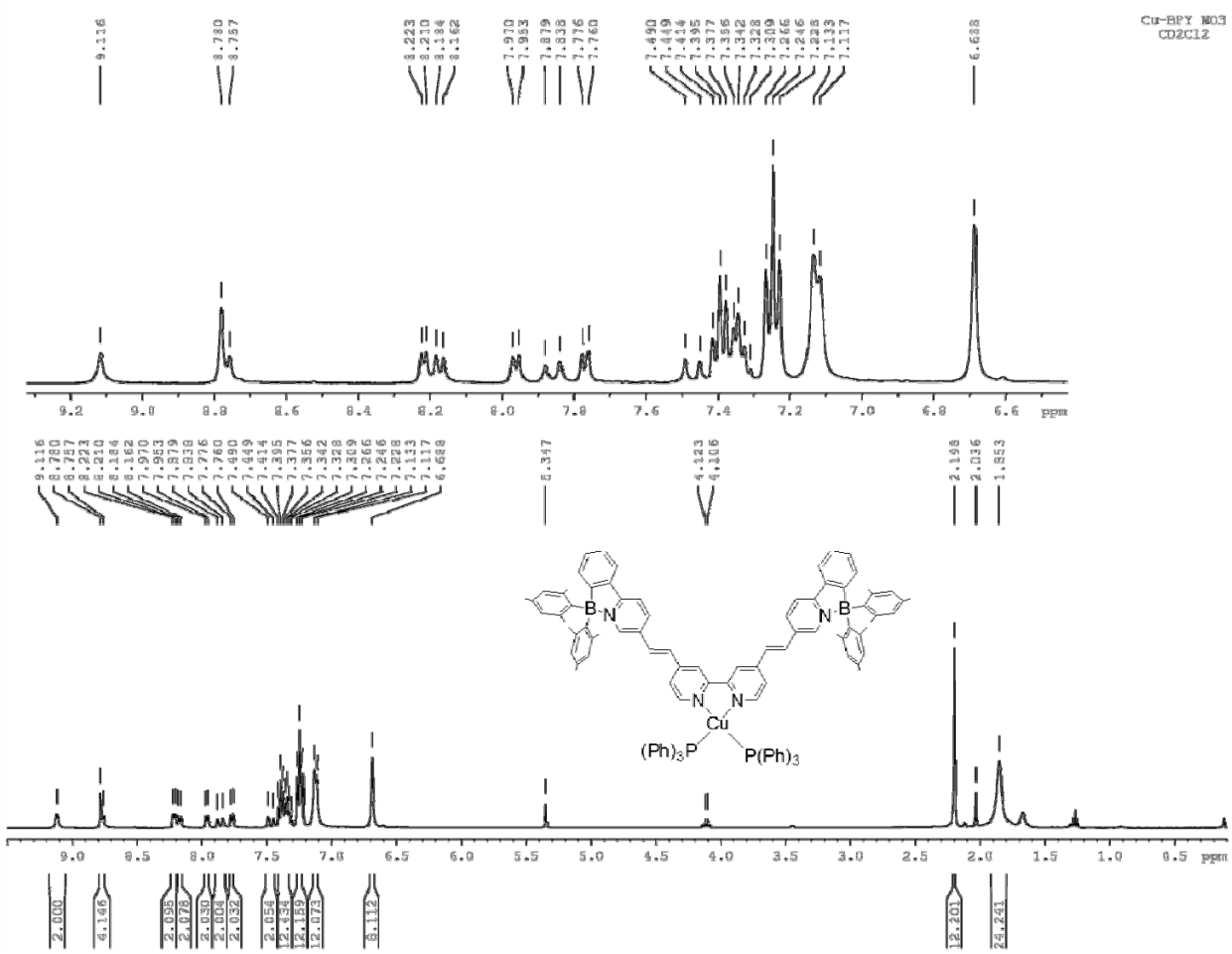
General procedures for NMR monitoring of the photolysis process : The photoisomerization was carried out by preparing a C_6D_6 (dried over NaH) solution (~0.03 M) in a NMR tube inside an inert atmosphere dry box. The solution was placed under UV (365 nm) at room temperature and the exposure time was recorded. After each exposure period, the NMR spectra were recorded.

General procedure for UV-Vis monitoring of the photolysis : The solution was prepared in the same manner as for NMR experiments except that the NMR tube was replaced by a UV cuvette that has a screw-on cap and the solution concentration is 10^{-5} M. The solvent used is toluene, freshly distilled.

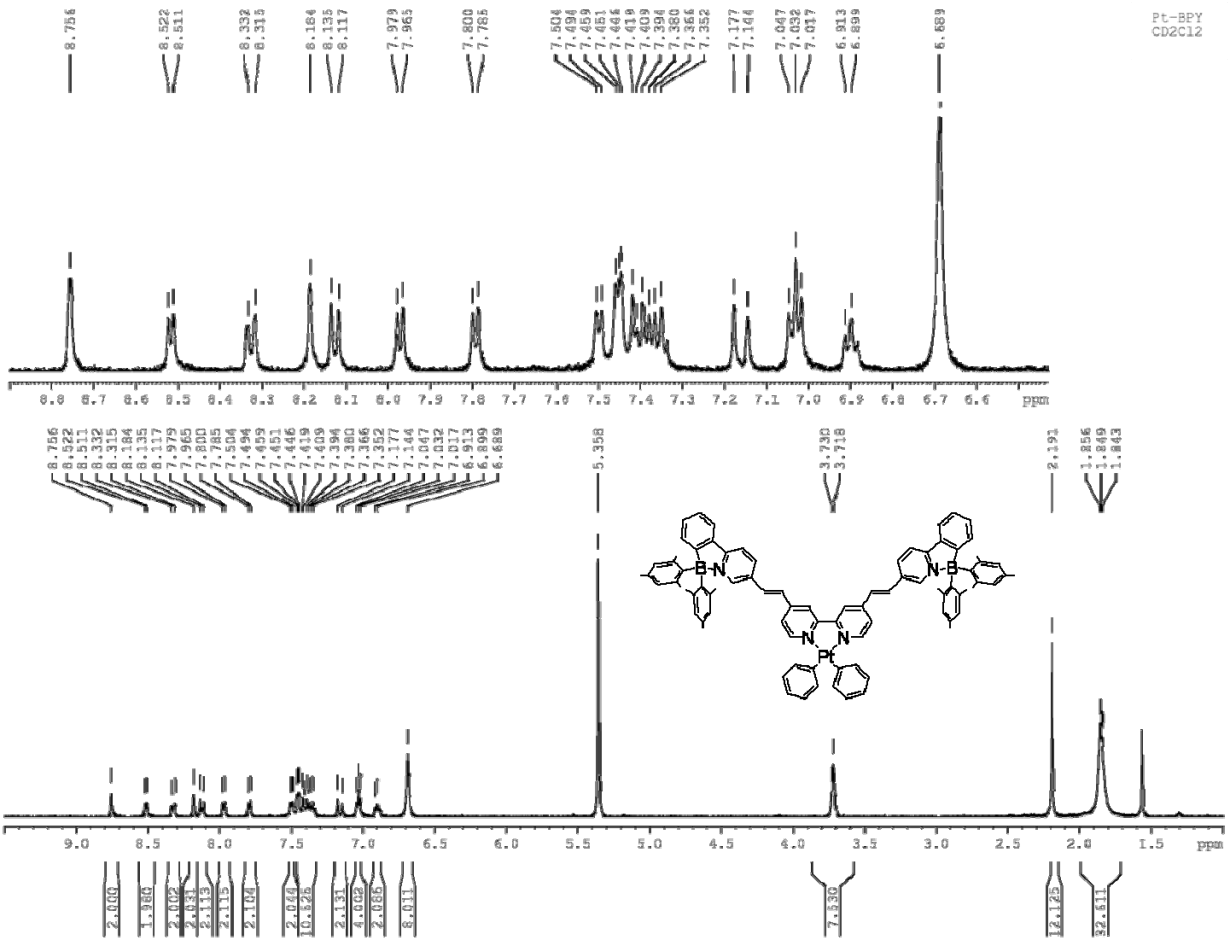
B-BPY. A solution of **1** (0.34 g, 0.80 mmol) and **2** (0.17, 0.36 mmol) in dry THF (15 mL) was added dropwise to a dry THF (10 mL) solution of K^{t}BuO (0.18 g, 1.6 mmol) at 0°C. The resulting reaction mixture was stirred for 5 h at room temperature and subsequently poured on brine. Organic phase was extracted with THF. Green solids of **B-BPY** were obtained from THF/Hx (83% yield). ^{1}H NMR (400 MHz, CD_2Cl_2): 8.69 (m, 4H), 8.59 (s, 2H), 8.28 (dd, *J* = 8.4, 1.6 Hz, 2H), 8.08 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 6.8 Hz, 2H), 7.77 (d, *J* = 6.8 Hz, 2H), 7.44 (dd, *J* = 5.2, 1.6 Hz, 2H), 7.36 (d, *J* = 16.4 Hz, 2H), 7.37-7.30 (m, 4H), 7.20 (d, *J* = 16.4 Hz, 2H), 6.68 (s, 8H), 2.19 (s, 12H), 1.84 (s, 24H); ^{13}C {^{1}H} NMR (400 MHz, CD_2Cl_2): 158.9, 156.8, 150.0, 145.3, 144.7, 140.5, 140.2, 137.6, 134.9, 134.2, 131.4, 131.1, 130.2, 129.8, 127.9, 125.7, 122.2, 121.5, 118.5, 118.4, 25.1, 20.6; HRMS, calcd. for $C_{72}H_{68}B_2N_4$: *m/z* 1011.5708; found: 1011.5700.



Cu-BPY. B-BPY (19.0 mg, 18.7 μmmol) and $[Cu(CH_3CN)_2(PPh_3)_2][BF_4]$ (12.1 mg, 18.7 μmmol) were mixed in 20 mL of CH_2Cl_2 and stirred for 12 h at room temperature. After removal of solvent, the yellow crude product recrystallized by ethyl acetate and methanol to afford **Cu-BPY** in 85% yield. ^{1}H NMR (400 MHz, CD_2Cl_2): 9.12 (s, 2H), 8.78 (s, 2H), 8.77 (d, J=8.8 Hz, 2H), 8.22 (d, J=5.2 Hz, 2H), 8.18 (d, J=8.8 Hz, 2H), 7.96 (d, J=6.8 Hz, 2H), 7.86 (d, J=16.4 Hz, 2H), 7.77 (d, J=6.8 Hz, 2H), 7.47 (d, J=16.4 Hz, 2H), 7.41-7.31 (m, 12H), 7.24 (t, J=8 Hz, 12H), 7.12 (m, 12H), 6.69 (s, 8H), 2.19 (s, 12H), 1.85 (s, 24H); ^{13}C {^{1}H} NMR (400 MHz, CD_2Cl_2): 159.1, 153.0, 149.4, 147.1, 145.9, 144.9, 140.2, 139.7, 135.2, 134.1, 133.4, 132.6, 131.4, 131.2, 130.9, 130.5, 130.1, 129.1, 127.9, 125.7, 122.8, 122.4, 121.9, 118.7, 25.1, 20.7. Anal. calcd for $C_{84}H_{78}B_2N_4Pt\cdot C_4H_8O_2$: C, 76.90; H, 6.11; N, 4.00. Found: C, 76.62; H, 6.05; N, 4.05.

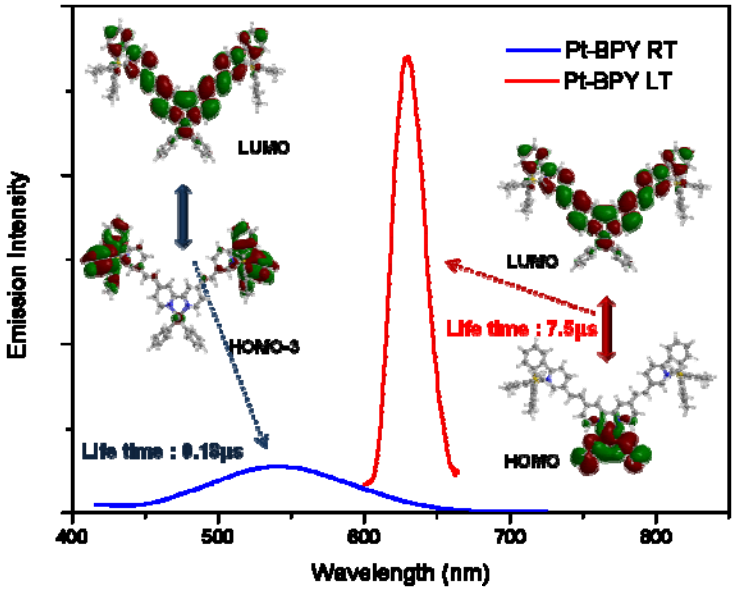


Pt-BPY. To a stirred THF (10 mL) solution of $[PtPh_2(SMe_2)]_2$ (32 mg, 0.037 mmol) was added **B-BPY** (50 mg, 0.050 mmol). The mixture was stirred at 50 °C for 6 h, and the solvent was removed under reduced pressure. Red needle crystals of **Pt-BPY** were obtained from toluene/Hx (70% yield). ^{1}H NMR (500 MHz, CD_2Cl_2): 8.76 (s, 2H), 8,52 (d, *J* = 5.5 Hz, 2H), 8.32 (d, *J* = 8.5 Hz, 2H), 8.18 (s, 2H), 8.12 (d, *J* = 8.5 Hz, 2H), 7.97 (d, *J* = 7.5 Hz, 2H), 7.79 (d, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 5 Hz, 2H), 7.49-7.34 (m, 10H), 7.16 (d, *J* = 16.5 Hz, 2H), 7.03 (m 4H), 6.90 (t, *J* = 7 Hz, 2H), 6.69 (s, 8H), 2.20 (s, 12H), 1.85 (s, 24H); ^{13}C {^{1}H} NMR (400 MHz, CD_2Cl_2): 159.5, 156.6, 150.5, 145.2, 145.2, 140.2, 138.5, 137.8, 134.9, 134.3, 131.8, 131.2, 130.4, 130.2, 128.1, 127.3, 125.9, 124.2, 122.5, 122.1, 120.1, 118.6, 25.1, 20.7. Anal. calcd for $C_{84}H_{78}B_2N_4Pt{\cdot}C_4H_8O$: C, 73.79; H, 6.05; N, 3.91. Found: C, 72.82; H, 5.54; N, 3.92.

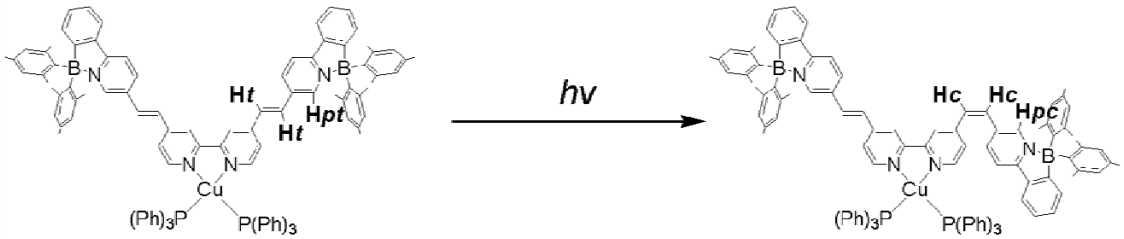


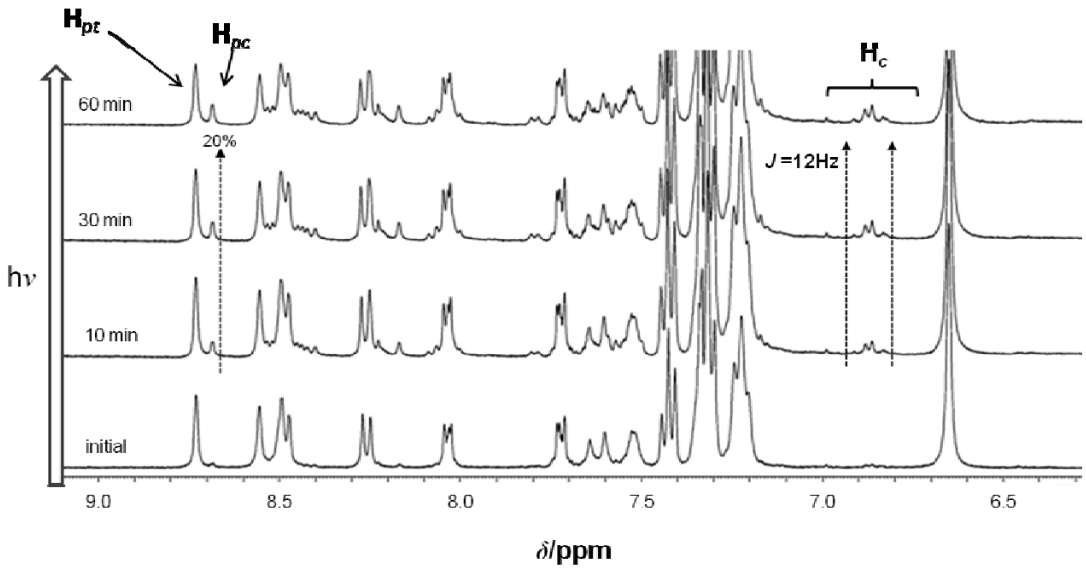
S2. Emission spectrum of Pt-BPY.

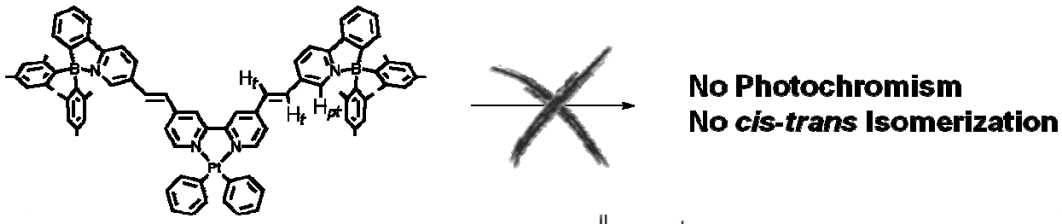
Emission spectrum of the Pt-BPY recorded in toluene (1.0 x 10^{-5} M) with at 390nm excitation wavelength for room temperature and 540nm for low temperature)

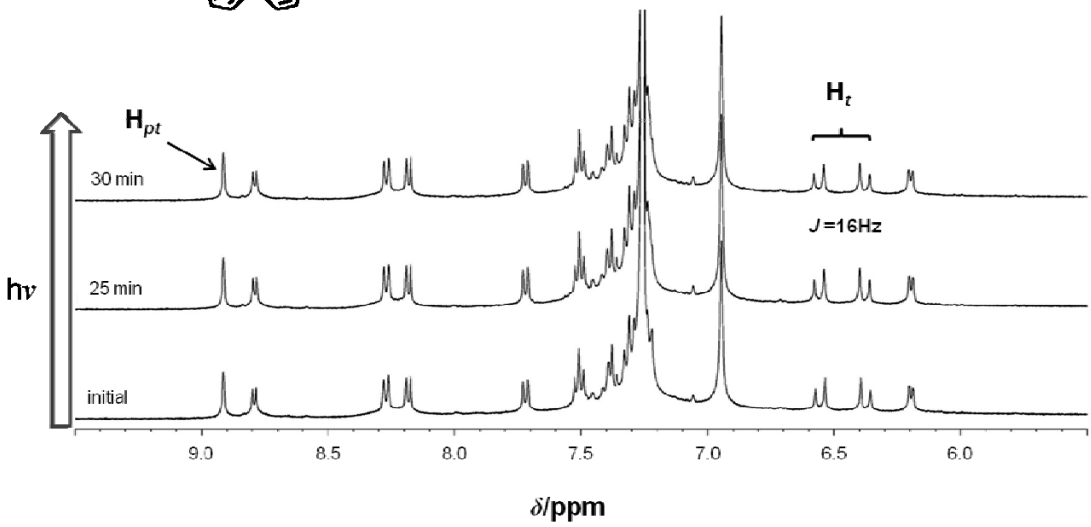


S3. ^{1}H NMR spectral change of Cu-BPY and Pt-BPY

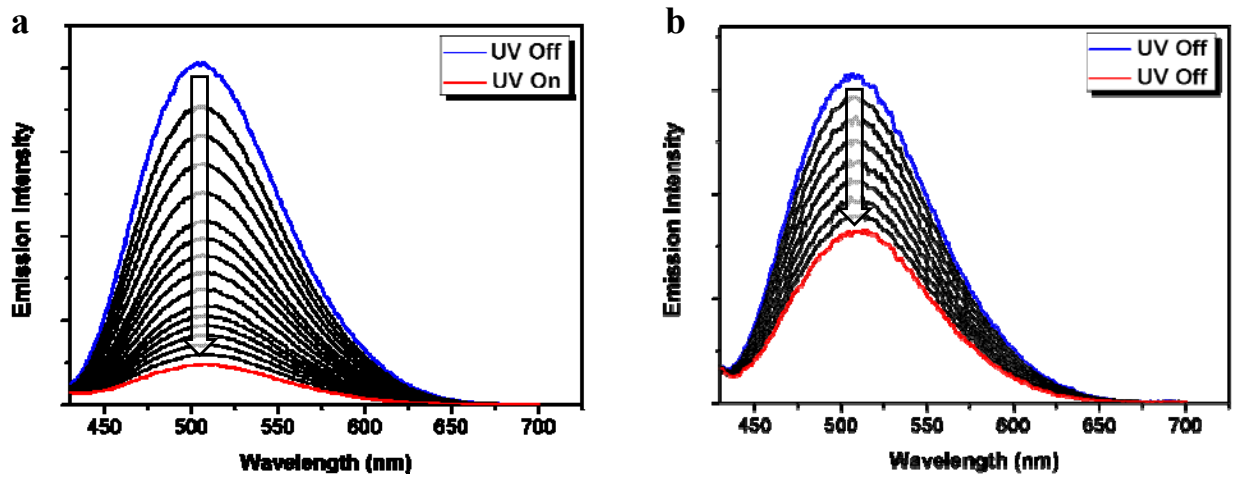








S4. Emission Spectral Change of B-BPY(a) and Cu-BPY(b).

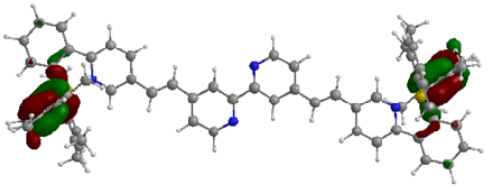
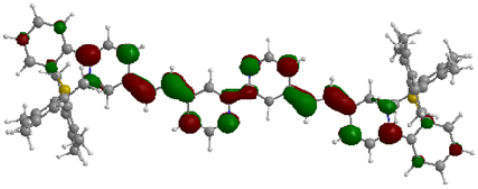
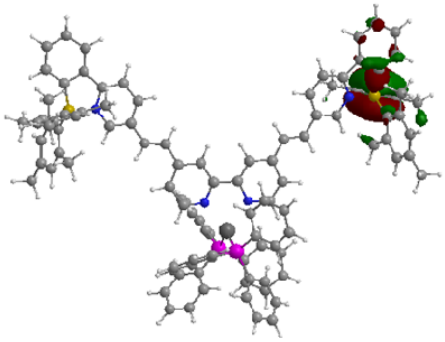
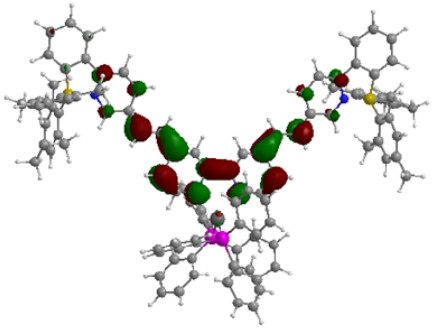
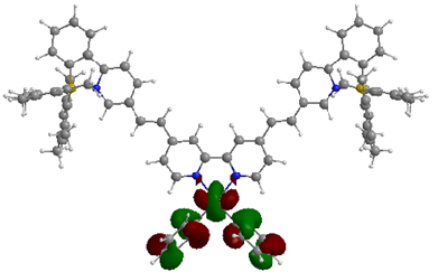
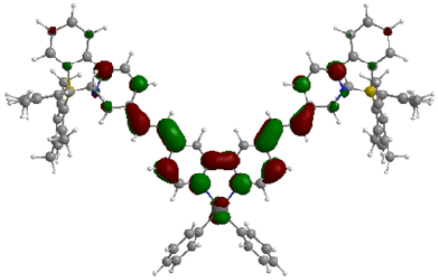


S5. Quantum Yield Measurement

Quantum yields of the compounds were determined in toluene using **Ir(PPy)$_3$** as the standard at 298 K (Φ_r = 0.97).[5] The absorbance of all the samples and the standard at the excitation wavelength is approximately 0.1 at 380 nm. The quantum yields were calculated using previously known procedures. The solution was prepared in the same manner as for UV-Vis monitoring of the photolysis in a UV cuvette that has a screw-on cap. The solvent used is toluene, freshly distilled.

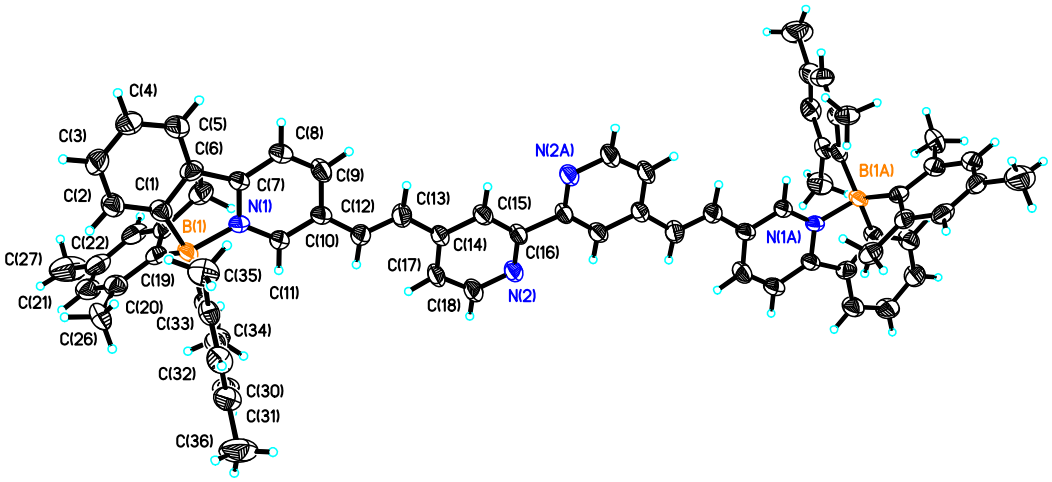
	B-BPY	Cu-BPY	Pt-BPY
Before Irradiation	0.69	0.12	≈0.001
After Irradiation	0.16	0.06	≈0.001

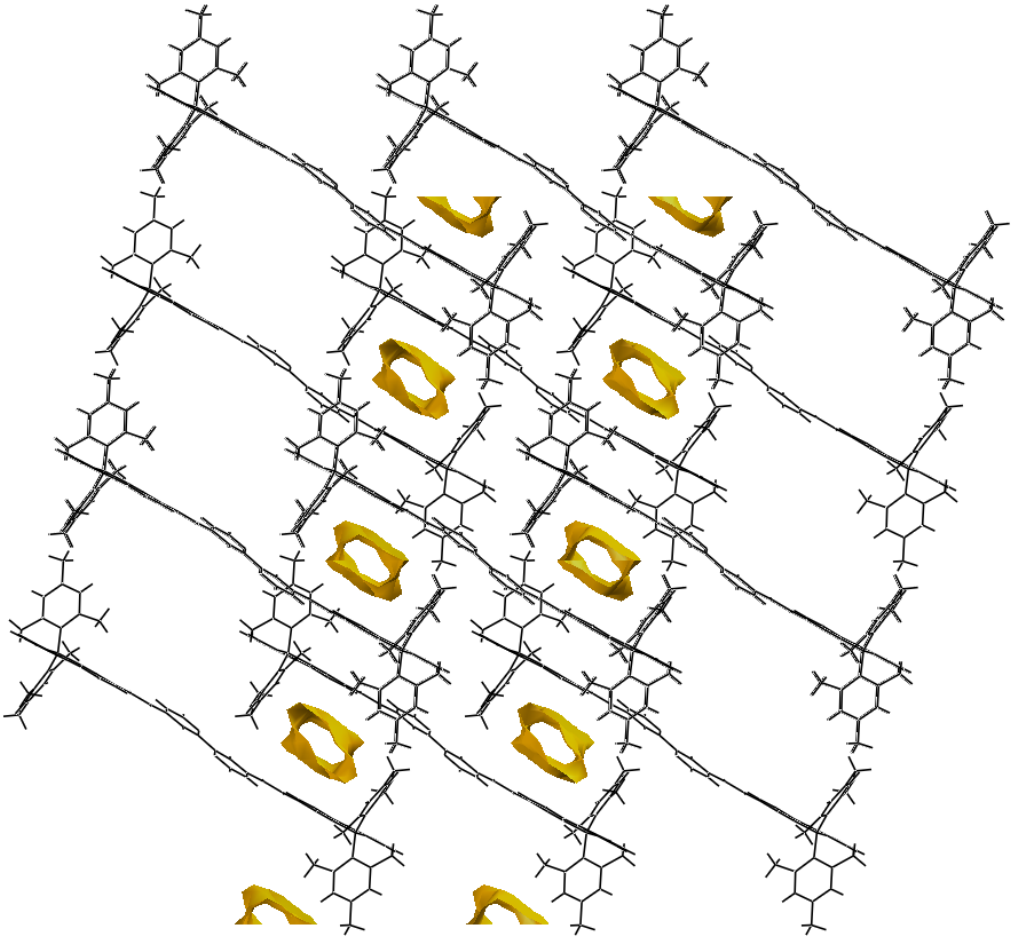
S6. DFT calculation results and HOMO-LUMO diagrams.

	HOMO	LUMO
B-BPY		
Cu-BPY		
Pt-BPY		

S7. Crystal Structural Data of B-BPY

Single-crystals of compound **B-BPY** was mounted on glass fibers in a brass pin, and the data was collected on a a Bruker AXS ApexII single-crystal X-ray diffractometer with graphitemonochromated Mo Kα radiation operating at 50 kV and 30 mA at 180 K. Data were processed on a Pentium PC using Bruker AXS SHELXTL software package. Empirical absorption correction was applied to all crystals. The crystals of compound **B-BPY** belongs to the Monoclinic space group C2/c. The structures were solved by direct methods The crystals contains disorded toluene solvent molecules (0.5 toluene/per molecule), which were removed by using the SQUEEZE routine of Platon.. All non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated, and their contributions in structural factor calculations were included.





The crystal lattice packing diagram projected down the *b*-axis showing the void space in the solvent channels

Table 1. Crystal data and structure refinement for baik12.

Identification code	baik12	
Empirical formula	C36 H34 B N2	
Formula weight	505.46	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 22.857(6) Å	□= 90°.
	b = 10.653(3) Å	□= 104.121(5)°.
	c = 28.098(7) Å	□ = 90°.
Volume	6635(3) $Å^3$	
Z	8	
Density (calculated)	1.012 Mg/m^3	
Absorption coefficient	0.058 mm^{-1}	
F(000)	2152	
Crystal size	0.20 x 0.20 x 0.05 mm^3	
Theta range for data collection	2.07 to 27.17°.	
Index ranges	-29<=h<=18, -11<=k<=13, -35<=l<=35	
Reflections collected	16111	
Independent reflections	7291 [R(int) = 0.1122]	
Completeness to theta = 27.17°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9971 and 0.9885	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7291 / 0 / 358	
Goodness-of-fit on F^2	0.797	
Final R indices [I>2sigma(I)]	R1 = 0.0785, wR2 = 0.1686	
R indices (all data)	R1 = 0.2270, wR2 = 0.2173	
Largest diff. peak and hole	0.261 and -0.279 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for baik12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	12467(2)	-1067(4)	8717(2)	34(1)
N(1)	12141(1)	-1568(3)	8163(1)	32(1)
N(2)	10336(1)	1480(3)	5230(1)	42(1)
C(1)	12554(2)	-2445(3)	8973(1)	38(1)
C(2)	12833(2)	-2863(4)	9442(1)	45(1)
C(3)	12884(2)	-4124(4)	9554(2)	53(1)
C(4)	12673(2)	-5019(4)	9202(2)	53(1)
C(5)	12410(2)	-4664(4)	8730(2)	50(1)
C(6)	12356(2)	-3378(3)	8622(1)	39(1)
C(7)	12086(2)	-2826(3)	8146(1)	37(1)
C(8)	11789(2)	-3405(3)	7707(1)	45(1)
C(9)	11552(2)	-2699(4)	7298(1)	44(1)
C(10)	11595(2)	-1386(3)	7318(1)	35(1)
C(11)	11892(2)	-883(3)	7765(1)	35(1)
C(12)	11358(2)	-566(3)	6906(1)	38(1)
C(13)	11065(2)	-917(4)	6458(1)	44(1)
C(14)	10828(2)	-71(3)	6041(1)	40(1)
C(15)	10454(2)	-542(3)	5609(1)	39(1)
C(16)	10209(2)	244(3)	5226(1)	35(1)
C(17)	10945(2)	1219(4)	6051(1)	48(1)
C(18)	10699(2)	1928(4)	5639(1)	50(1)
C(19)	13157(2)	-531(3)	8789(1)	37(1)
C(20)	13425(2)	107(3)	9232(2)	43(1)
C(21)	14015(2)	579(4)	9322(2)	52(1)
C(22)	14361(2)	430(4)	8996(2)	53(1)
C(23)	14128(2)	-242(3)	8566(2)	49(1)
C(24)	13538(2)	-722(3)	8464(1)	37(1)
C(25)	13347(2)	-1464(3)	7991(1)	47(1)
C(26)	13101(2)	351(4)	9630(1)	58(1)
C(27)	15007(2)	945(4)	9096(2)	93(2)
C(28)	11981(2)	-37(3)	8830(1)	36(1)

C(29)	12016(2)	1248(3)	8710(1)	38(1)
C(30)	11618(2)	2122(4)	8837(2)	50(1)
C(31)	11178(2)	1792(4)	9068(2)	53(1)
C(32)	11115(2)	523(4)	9155(1)	47(1)
C(33)	11494(2)	-385(4)	9032(1)	39(1)
C(34)	12461(2)	1789(3)	8441(1)	44(1)
C(35)	11349(2)	-1741(3)	9131(2)	56(1)
C(36)	10770(2)	2775(4)	9207(2)	86(2)

Table 3. Bond lengths [Å] and angles [°] for baik12.

B(1)-C(1)	1.625(5)	C(14)-C(17)	1.399(5)
B(1)-C(19)	1.641(6)	C(15)-C(16)	1.371(5)
B(1)-N(1)	1.642(5)	C(16)-C(16)#1	1.484(6)
B(1)-C(28)	1.648(5)	C(17)-C(18)	1.381(5)
N(1)-C(11)	1.341(4)	C(19)-C(20)	1.421(5)
N(1)-C(7)	1.346(4)	C(19)-C(24)	1.422(5)
N(2)-C(18)	1.332(4)	C(20)-C(21)	1.402(5)
N(2)-C(16)	1.348(4)	C(20)-C(26)	1.507(5)
C(1)-C(2)	1.391(5)	C(21)-C(22)	1.358(6)
C(1)-C(6)	1.395(5)	C(22)-C(23)	1.393(6)
C(2)-C(3)	1.378(5)	C(22)-C(27)	1.536(6)
C(3)-C(4)	1.373(5)	C(23)-C(24)	1.405(5)
C(4)-C(5)	1.367(5)	C(24)-C(25)	1.515(5)
C(5)-C(6)	1.402(5)	C(28)-C(29)	1.416(5)
C(6)-C(7)	1.454(5)	C(28)-C(33)	1.417(5)
C(7)-C(8)	1.398(5)	C(29)-C(30)	1.407(5)
C(8)-C(9)	1.371(5)	C(29)-C(34)	1.522(5)
C(9)-C(10)	1.402(5)	C(30)-C(31)	1.369(5)
C(10)-C(11)	1.382(5)	C(30)-H(30A)	0.9500
C(10)-C(12)	1.446(5)	C(31)-C(32)	1.388(5)
C(12)-C(13)	1.328(5)	C(31)-C(36)	1.515(5)
C(13)-C(14)	1.473(5)	C(32)-C(33)	1.396(5)
C(14)-C(15)	1.396(4)	C(33)-C(35)	1.522(5)

C(1)-B(1)-C(19)	104.5(3)
C(1)-B(1)-N(1)	95.9(3)
C(19)-B(1)-N(1)	115.4(3)
C(1)-B(1)-C(28)	122.2(3)
C(19)-B(1)-C(28)	114.7(3)
N(1)-B(1)-C(28)	103.1(3)
C(11)-N(1)-C(7)	119.7(3)
C(11)-N(1)-B(1)	128.0(3)
C(7)-N(1)-B(1)	112.0(3)
C(18)-N(2)-C(16)	116.4(3)
C(2)-C(1)-C(6)	115.9(3)
C(2)-C(1)-B(1)	133.4(3)
C(6)-C(1)-B(1)	110.4(3)
C(3)-C(2)-C(1)	121.4(4)
C(3)-C(2)-H(2A)	119.3
C(1)-C(2)-H(2A)	119.3
C(4)-C(3)-C(2)	121.2(4)
C(4)-C(3)-H(3A)	119.4
C(2)-C(3)-H(3A)	119.4
C(5)-C(4)-C(3)	120.0(4)
C(5)-C(4)-H(4A)	120.0
C(3)-C(4)-H(4A)	120.0
C(4)-C(5)-C(6)	118.3(4)
C(4)-C(5)-H(5A)	120.8
C(6)-C(5)-H(5A)	120.8
C(1)-C(6)-C(5)	123.2(3)
C(1)-C(6)-C(7)	110.7(3)
C(5)-C(6)-C(7)	126.1(4)
N(1)-C(7)-C(8)	119.5(3)
N(1)-C(7)-C(6)	110.8(3)
C(8)-C(7)-C(6)	129.7(3)
C(9)-C(8)-C(7)	120.4(3)
C(9)-C(8)-H(8A)	119.8
C(7)-C(8)-H(8A)	119.8
C(8)-C(9)-C(10)	120.2(3)
C(8)-C(9)-H(9A)	119.9
C(10)-C(9)-H(9A)	119.9
C(11)-C(10)-C(9)	116.0(3)
C(11)-C(10)-C(12)	119.9(3)
C(9)-C(10)-C(12)	124.1(3)
N(1)-C(11)-C(10)	124.2(3)
N(1)-C(11)-H(11A)	117.9
C(10)-C(11)-H(11A)	117.9
C(13)-C(12)-C(10)	126.3(4)
C(13)-C(12)-H(12A)	116.8
C(10)-C(12)-H(12A)	116.8
C(12)-C(13)-C(14)	125.7(4)
C(12)-C(13)-H(13A)	117.1
C(14)-C(13)-H(13A)	117.1
C(15)-C(14)-C(17)	116.4(3)
C(15)-C(14)-C(13)	120.0(3)
C(17)-C(14)-C(13)	123.7(3)
C(16)-C(15)-C(14)	120.6(3)
C(16)-C(15)-H(15A)	119.7
C(14)-C(15)-H(15A)	119.7
N(2)-C(16)-C(15)	123.0(3)
N(2)-C(16)-C(16)#1	116.2(4)
C(15)-C(16)-C(16)#1	120.8(4)
C(18)-C(17)-C(14)	118.9(3)
C(18)-C(17)-H(17A)	120.5
C(14)-C(17)-H(17A)	120.5
N(2)-C(18)-C(17)	124.6(4)
N(2)-C(18)-H(18A)	117.7
C(17)-C(18)-H(18A)	117.7
C(20)-C(19)-C(24)	115.5(3)
C(20)-C(19)-B(1)	118.1(4)
C(24)-C(19)-B(1)	126.3(3)

C(21)-C(20)-C(19)	121.4(4)	C(29)-C(28)-B(1)	121.2(3)
C(21)-C(20)-C(26)	115.3(4)	C(33)-C(28)-B(1)	122.4(3)
C(19)-C(20)-C(26)	123.2(4)	C(30)-C(29)-C(28)	120.1(4)
C(22)-C(21)-C(20)	121.9(4)	C(30)-C(29)-C(34)	115.3(3)
C(22)-C(21)-H(21A)	119.1	C(28)-C(29)-C(34)	124.6(3)
C(20)-C(21)-H(21A)	119.1	C(31)-C(30)-C(29)	123.0(4)
C(21)-C(22)-C(23)	118.9(4)	C(31)-C(30)-H(30A)	118.5
C(21)-C(22)-C(27)	121.8(4)	C(29)-C(30)-H(30A)	118.5
C(23)-C(22)-C(27)	119.3(5)	C(30)-C(31)-C(32)	116.9(4)
C(22)-C(23)-C(24)	120.6(4)	C(30)-C(31)-C(36)	120.9(4)
C(22)-C(23)-H(23A)	119.7	C(32)-C(31)-C(36)	122.2(4)
C(24)-C(23)-H(23A)	119.7	C(31)-C(32)-C(33)	122.3(4)
C(23)-C(24)-C(19)	121.6(4)	C(31)-C(32)-H(32A)	118.8
C(23)-C(24)-C(25)	115.2(4)	C(33)-C(32)-H(32A)	118.8
C(19)-C(24)-C(25)	123.2(3)	C(32)-C(33)-C(28)	120.8(3)
C(24)-C(25)-H(25A)	109.5	C(32)-C(33)-C(35)	115.9(4)
C(24)-C(25)-H(25B)	109.5	C(28)-C(33)-C(35)	123.3(4)
H(25A)-C(25)-H(25B)	109.5	C(29)-C(34)-H(34A)	109.5
C(24)-C(25)-H(25C)	109.5	C(29)-C(34)-H(34B)	109.5
H(25A)-C(25)-H(25C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(25B)-C(25)-H(25C)	109.5	C(29)-C(34)-H(34C)	109.5
C(20)-C(26)-H(26A)	109.5	H(34A)-C(34)-H(34C)	109.5
C(20)-C(26)-H(26B)	109.5	H(34B)-C(34)-H(34C)	109.5
H(26A)-C(26)-H(26B)	109.5	C(33)-C(35)-H(35A)	109.5
C(20)-C(26)-H(26C)	109.5	C(33)-C(35)-H(35B)	109.5
H(26A)-C(26)-H(26C)	109.5	H(35A)-C(35)-H(35B)	109.5
H(26B)-C(26)-H(26C)	109.5	C(33)-C(35)-H(35C)	109.5
C(22)-C(27)-H(27A)	109.5	H(35A)-C(35)-H(35C)	109.5
C(22)-C(27)-H(27B)	109.5	H(35B)-C(35)-H(35C)	109.5
H(27A)-C(27)-H(27B)	109.5	C(31)-C(36)-H(36A)	109.5
C(22)-C(27)-H(27C)	109.5	C(31)-C(36)-H(36B)	109.5
H(27A)-C(27)-H(27C)	109.5	H(36A)-C(36)-H(36B)	109.5
H(27B)-C(27)-H(27C)	109.5	C(31)-C(36)-H(36C)	109.5
C(29)-C(28)-C(33)	116.4(3)	H(36A)-C(36)-H(36C)	109.5

H(36B)-C(36)-H(36C) 109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for baik12. 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)	44(3)	25(2)	31(2)	-6(2)	4(2)	-5(2)
N(1)	37(2)	22(2)	35(2)	-1(1)	8(2)	1(1)
N(2)	45(2)	35(2)	39(2)	-3(2)	-2(2)	-7(2)
C(1)	42(2)	32(2)	38(2)	-3(2)	9(2)	-7(2)
C(2)	59(3)	38(2)	37(2)	1(2)	7(2)	-4(2)
C(3)	63(3)	42(3)	47(3)	10(2)	0(2)	2(2)
C(4)	69(3)	32(2)	55(3)	7(2)	11(2)	-1(2)
C(5)	63(3)	34(3)	49(3)	-2(2)	4(2)	-4(2)
C(6)	44(2)	26(2)	45(2)	6(2)	9(2)	2(2)
C(7)	46(2)	28(2)	34(2)	-5(2)	4(2)	1(2)
C(8)	54(3)	29(2)	48(3)	-7(2)	5(2)	-3(2)
C(9)	51(3)	47(3)	30(2)	-6(2)	4(2)	-5(2)
C(10)	42(2)	26(2)	36(2)	-3(2)	7(2)	-1(2)
C(11)	40(2)	29(2)	33(2)	-2(2)	3(2)	2(2)
C(12)	41(2)	34(2)	36(2)	1(2)	2(2)	-1(2)
C(13)	45(2)	39(2)	41(2)	3(2)	-3(2)	-6(2)
C(14)	43(2)	35(2)	34(2)	-5(2)	-3(2)	-3(2)
C(15)	46(2)	33(2)	35(2)	-4(2)	3(2)	-6(2)
C(16)	39(2)	35(2)	27(2)	-4(2)	2(2)	-7(2)
C(17)	55(3)	40(3)	37(2)	-5(2)	-11(2)	-9(2)
C(18)	49(3)	41(3)	49(3)	-7(2)	-8(2)	-10(2)
C(19)	43(2)	24(2)	41(2)	4(2)	4(2)	5(2)
C(20)	44(2)	31(2)	52(3)	-2(2)	8(2)	-3(2)

C(21)	43(3)	35(2)	71(3)	-10(2)	3(2)	-1(2)
C(22)	32(2)	31(2)	88(4)	1(2)	1(2)	2(2)
C(23)	37(2)	32(2)	76(3)	6(2)	11(2)	6(2)
C(24)	41(2)	27(2)	39(2)	10(2)	4(2)	3(2)
C(25)	51(3)	44(2)	49(3)	9(2)	16(2)	7(2)
C(26)	60(3)	65(3)	41(3)	-16(2)	-4(2)	-5(2)
C(27)	52(3)	54(3)	172(6)	-25(3)	26(3)	-12(3)
C(28)	37(2)	34(2)	31(2)	-6(2)	-1(2)	-5(2)
C(29)	35(2)	31(2)	44(2)	-7(2)	1(2)	-5(2)
C(30)	55(3)	34(2)	60(3)	-5(2)	14(2)	4(2)
C(31)	46(3)	52(3)	62(3)	-15(2)	16(2)	-3(2)
C(32)	35(2)	59(3)	50(3)	-8(2)	16(2)	-10(2)
C(33)	38(2)	44(3)	34(2)	-2(2)	6(2)	-11(2)
C(34)	53(3)	28(2)	54(3)	4(2)	20(2)	-3(2)
C(35)	61(3)	47(3)	66(3)	1(2)	26(2)	-11(2)
C(36)	74(3)	75(4)	118(5)	-31(3)	41(3)	15(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for baik12.

	x	y	z	U(eq)
H(2A)	12991	-2266	9692	55
H(3A)	13068	-4379	9880	63
H(4A)	12710	-5884	9286	64
H(5A)	12267	-5274	8483	60
H(8A)	11750	-4293	7693	54
H(9A)	11358	-3100	6999	52
H(11A)	11920	5	7792	42
H(12A)	11419	310	6962	46
H(13A)	11004	-1792	6401	53
H(15A)	10369	-1416	5580	47

H(17A)	11191	1601	6336	57
H(18A)	10795	2797	5649	60
H(21A)	14176	1016	9620	62
H(23A)	14371	-377	8340	58
H(25A)	13697	-1591	7852	71
H(25B)	13034	-1000	7756	71
H(25C)	13187	-2280	8059	71
H(26A)	13383	242	9952	87
H(26B)	12766	-241	9597	87
H(26C)	12945	1211	9600	87
H(27A)	15136	1218	9439	139
H(27B)	15018	1660	8879	139
H(27C)	15278	286	9035	139
H(30A)	11656	2981	8759	60
H(32A)	10804	262	9303	56
H(34A)	12256	2416	8202	66
H(34B)	12616	1113	8268	66
H(34C)	12797	2185	8677	66
H(35A)	10980	-1768	9249	85
H(35B)	11684	-2099	9380	85
H(35C)	11291	-2229	8827	85
H(36A)	10947	3609	9194	129
H(36B)	10729	2612	9540	129
H(36C)	10372	2740	8976	129

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