2,2′-Bipyridinyl Carboranes as *B,N,N*-ligands in Cyclometallated Complexes of Platinum(II)

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Electronic Supplimentary Information (ESI)

General Information

All chemicals and solvents were used as supplied, unless noted otherwise. The ligands were prepared according to following procedure or were described earlier (see references).

Absorption spectra were measured on a Shimadzu UV-2450 spectrometer, using quartz cuvettes of 1 cm pathlength. Steady-state luminescence spectra were measured using a Varian Cary Eclipse spectrofluorimeter. De-aerating was achieved by bubbling argon through the solution for 10 min. Measurements at 77 K were recorded using a Oxford Instruments Optistat DN cryostat with the sample held in 4 mm o.d. quartz tubes.

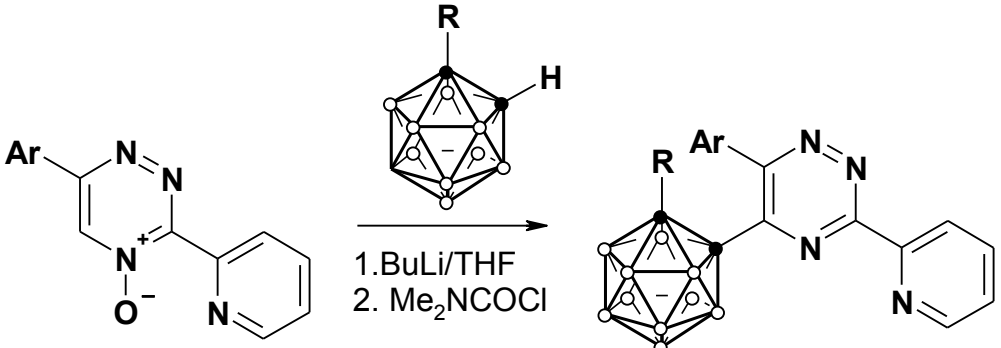
The ^{1}H- and ^{13}C NMR spectra were recorded using a Bruker Avans II 400 running Delta (400 MHz for ^{1}H; 100 MHz for ^{13}C). Data are expressed in parts per million downfield shift from tetramethylsilane as an internal standard or relative to $CDCl_3$. All *J* values are given in Hz. Assignments are made with the calculation of the constant coupling.

Mass spectra were recorded using a Bruker Daltronics microTOF spectrometer operating in electrospray ionisation (ESI) mode.

Values were obtained in Insitute of Organic Synthesis, Russian Academy of Science, Kovalevskoy 20, Ekaterinburg, on CE-440 Elemental Analyser. Calibration performed against acetanilide standards and checked by the use of *S*-benzyl thiouronium chloride as internal standard. Carrier gas is CP-grade Helium and combustion gas is N5.5 grade Oxygen, both from BOC.

Ligand Preparation

General procedure for preparation of 1-(3,6-disubstituted-1,2,4-triazine-5-yl)-1,2-dicarba-*closo*-dodecaboranes (5):



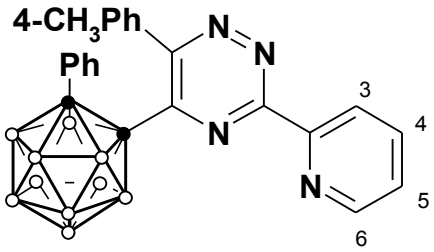
4a,b **5a,b**

A 1.6 M solution of *n*-butyllithium in pentane (1.10 mmol, 0.69 mL) was added to a solution of corresponding carborane (1.20 mmol) in dry THF (20 mL) at room temperature under argon atmosphere. The resulting solution of carboranyllithium was added dropwise to a suspension of corresponding 6-aryl-1,2,4-triazine 4-oxide[1] **4** (1 mmol) in dry THF (15 mL) at –40 °C, and the mixture was stirred and allowed slowly . When the mixture had become a clear solution, dimethylcarbamyl chloride (1.1 mmol, 0.101 mL) was added. The solvent was removed, and the residue was treated with hot toluene (40 mL). The toluene solution was separated from solids by

[1] Kozhevnikov, V. N.; Kozhevnikov, D. N.; Nikitina, T. V.; Rusinov, V. L.; Chupakhin, O. N.; Zabel, M.; Koenig., B. *J. Org. Chem.* **2003**, *68*, 2882.

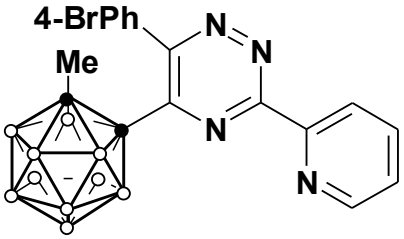
filtration, and the solvent was removed. The residue was dissolved in acetonitrile (10 mL) and cooled down in a fridge to form yellow crystals of triazinyl carborane **5** which were filtered off.

1-[6-(4-Methylphenyl)-3-(2-pyridyl)-1,2,4-triazine-5-yl]-2-phenyl-1,2-dicarba-*closo*-dodecaborane (5a):



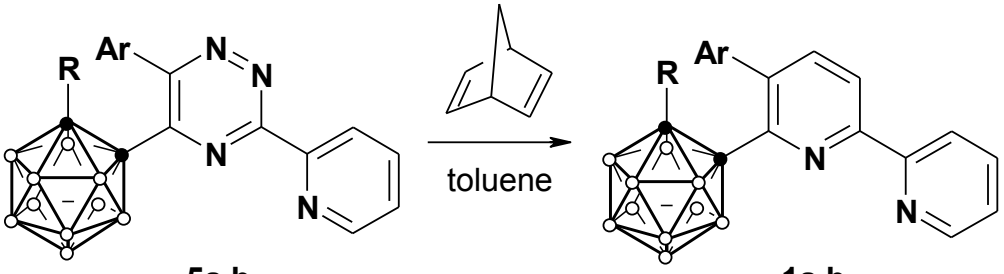
Yield 210 mg, 45%. M.p. 171 °C. ^{1}H NMR ($CDCl_3$), δ: 8.92 (1H, d, ^{3}J = 4.5 Hz, Py^{6}), 8.42 (1H, d, ^{3}J = 8.0 Hz, Py^{3}), 7.97 (1H, dd, $^{3}J_1$ = $^{3}J_2$ = 8.0 Hz, Py^{4}), 7.58-7.54 (3H, m, Tol+Py^{5}), 7.08 (2H, m, Tol), 2.46 (3H, s, CH_3), 1.20–3.40 (br.m, 10H, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –1.4 (2B), –3.5 (2B), –10.3 (6B). Anal. Calcd for $C_{23}H_{26}B_{10}N_4$: C, 59.21; H, 5.62; N, 12.10. Found: C, 59.33; H, 5.56; N, 12.26.

1-[6-(4-Bromophenyl)-3-(2-pyridyl)-1,2,4-triazine-5-yl]-2-methyl-1,2-dicarba-*closo*-dodecaborane (5b):



Yield 255 mg, 54%. M.p. 167 °C. ^{1}H NMR ($CDCl_3$), δ: 8.95 (1H, d, ^{3}J = 4.5 Hz, Py^{6}), 8.57 (1H, d, ^{3}J = 8.0 Hz, Py^{3}), 7.99 (1H, dd, $^{3}J_1$ = $^{3}J_2$ = 8.0 Hz, Py^{4}), 7.71 (2H, m, Ar), 7.56 (1H, dd, $^{3}J_1$ = 4.5, $^{3}J_2$ = 8.0 Hz, Py^{5}), 7.37 (2H, m, Ar), 1.85 (3H, s, CH_3), 3.20–1.40 (br.m, 10H, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –1.6 (2B), –3.7 (2B), –10.4 (6B). Anal. Calcd for $C_{17}H_{21}B_{10}BrN_4$: C, 43.50; H, 4.51; N, 11.94. Found: C, 43.33; H, 5.48; N, 11.96.

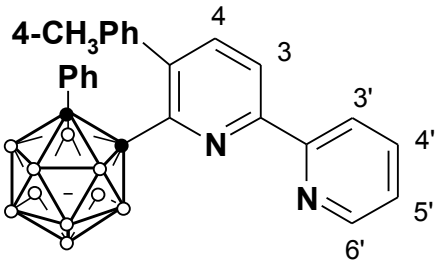
General procedure for preparation of bipyridyl carboranes (1):



5a,b **1a,b**

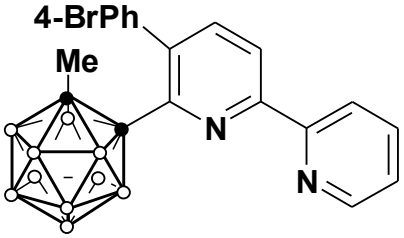
A triazinyl carborane **5** (0.5 mmol) and 2,5-norbornadiene (0.27 mL, 2.5 mmol) were dissolved in toluene (20 mL) and stirred under reflux for 5 h. Then solvent was removed under reduced pressure, and the residue was treated with acetonitrile (10 mL) to form colorless crystals of bipyridyl carborane **1** which were filtered off.

1-[5-(4-Methylphenyl)-2,2′-bipyridine-6-yl]-2-phenyl-1,2-dicarba-*closo*-dodecaborane (1a):



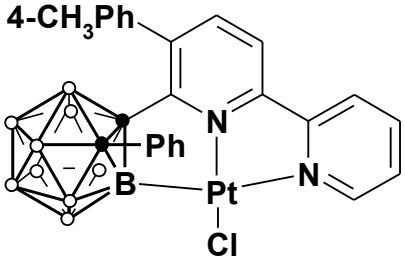
Yield 209 mg, 90%. M.p. 183 °C. ^{1}H NMR ($CDCl_3$), δ: 8.67 (1H, d, ^{3}J = 4.0 Hz, H6′), 8.53 (1H, d, ^{3}J = 8.0 Hz, H3′), 8.26 (1H, d, ^{3}J = 8.0 Hz, H4), 7.93 (1H, dd, $^{3}J_1$ = 7.5, $^{3}J_2$ = 8.0 Hz, H4′), 7.38 (1H, dd, $^{3}J_1$ = 7.5, $^{3}J_2$ = 4.0 Hz, H5′), 7.32 (1H, d, ^{3}J = 8.0 Hz, H3), 7.28-7.06 (7H, m, Ar), 6.66 (2H, m, Ar), 2.45 (3H, s, CH_3), 1.50–3.50 (br.m, 10H, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –1.6 (2B), –3.7 (2B), –10.5 (6B). Anal. Calcd for $C_{25}H_{28}B_{10}N_2$: C, 64.63; H, 6.07; N, 6.03. Found: C, 64.79; H, 5.98; N, 5.99.

1-[5-(4-Bromophenyl)-2,2'-bipyridine-6-yl]-2-methyl-1,2-dicarba-*closo*-dodecaborane (1b):



Yield 205 mg, 88%. M.p. 177 °C. ^{1}H NMR ($CDCl_3$), δ: 8.68 (1H, d, ^{3}J = 4.0 Hz, H6′), 8.55 (1H, d, ^{3}J = 8.0 Hz, H3′), 8.25 (1H, d, ^{3}J = 8.0 Hz, H4), 7.95 (1H, dd, $^{3}J_1$ = 7.5, $^{3}J_2$ = 8.0 Hz, H4′), 7.56 (2H, m, Ar), 7.41 (1H, dd, $^{3}J_1$ = 7.5, $^{3}J_2$ = 4.0 Hz, H5′), 7.35 (1H, d, ^{3}J = 8.0 Hz, H3), 7.30 (2H, m, Ar), 1.88 (3H, s, CH_3), 1.50–3.50 (br.m, 10H, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –1.4 (2B), –3.6 (2B), –10.1 (6B). Anal. Calcd for $C_{19}H_{23}B_{10}BrN_2$: C, 48.82; H, 4.96; N, 5.99. Found: C, 48.73; H, 5.01; N, 5.86.

Complex 2a:

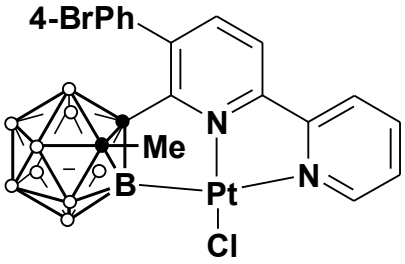


Bipyridinyl carborane **1a** (250 mg, 0.54 mmol) was dissolved in boiling acetonitrile (20 mL), and a water solution (5 mL) of potassium tetrachloroplatinate (223 mg, 0.54 mmol) was added to the mixture. This was stirred and refluxed for 72 h with control of consumption of starting material by TLC. After reaction was completed the solvent was removed and complex **2a** was isolated by coloumn chromatography on silica (eluent – ethylacetate). The product was purified by crystallization from acetonitrile to give yellow crystals of **2a**. A single crystal for X-ray analysis was grown by slow evaporation of acetonitrile solution. Yield 53% (200 mg, 0.29 mmol). ^{1}H NMR ($CDCl_3$), δ: 9.19 (1H, dd, ^{3}J = 5.0, ^{4}J = 1.0 Hz, H6′), 8.07 (3H, m, H4′+Ar), 7.97 (1H, d, ^{3}J = 8.0 Hz, H3′), 7.86 (1H, d, ^{3}J = 8.0 Hz, H4), 7.78 (1H, dd, $^{3}J_1$ = 8.0, $^{3}J_2$ = 5.0, Hz, H5′), 7.74 (1H, ^{3}J = 8.0 Hz, H3), 7.38 (1H, m, Ar), 7.39-7.21 (4H, m, Ar), 7.10-7.04 (3H, m, Ar), 2.52 (3H, s, Me), 3.40-1.60 (9H, br.m, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –0.3 (2B), –3.7 (2B), –5.2 (1B), –8.9 (2B), –10.8 (1B), –12.4 (1B). ESI-MS, m/z: found 695.2547, calcd. 695.2573 for $C_{25}H_{27}B_{10}ClN_2Pt$.

X-ray data: A single crystal for X-ray analysis was grown by slow evaporation of

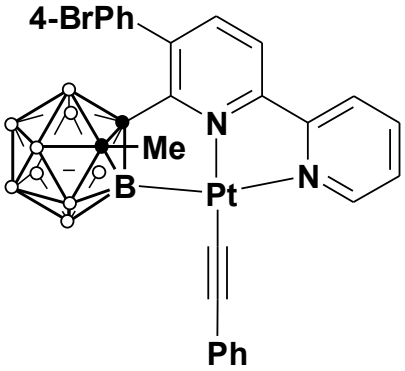
acetonitrile solution.

Complex 2b:



Bipyridinyl carborane **1b** (250 mg, 0.54 mmol) was dissolved in boiling acetonitrile (20 mL), and a water solution (5 mL) of potassium tetrachloroplatinate (222 mg, 0.54 mmol) was added to the mixture. This was stirred and refluxed for 72 h with control of consumption of starting material by TLC. After reaction was completed the solvent was removed and complex **2b** was isolated by coloumn chromatography on silica (eluent – ethylacetate). The product was purified by crystallization from acetonitrile to give yellow crystals of **2b**. Yield 46% (175 mg, 0.25 mmol). ^{1}H NMR ($CDCl_3$), δ: 9.32 (1H, dd, ^{3}J = 4.5, ^{4}J = 1.0 Hz, H6′), 8.18 (2H, m, H4′+ H3′), 7.97 (2H, m, H3+H4), 7.90 (1H, dd, $^{3}J_1$ = 8.0, $^{3}J_2$ = 5.0, Hz, H5′), 7.62 (2H, m, Ar), 7.22 (1H, m, Ar), 7.03 (1H, m, Ar), 1.96 (3H, s, Me), 3.40-1.60 (9H, br.m, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –0.3 (2B), –3.4 (2B), –5.2 (1B), –8.3 (2B), –10.2 (1B), –12.3 (1B). ESI-MS, m/z: found 697.1267, calcd. 697.1223 for $C_{19}H_{22}B_{10}BrClN_2Pt$.

Complex 3b:



Complex **2b** (100 mg, 0.14 mmol) was dissolved in boiling acetonitrile, and anhydrous potassium carbonate and phenylacetylene were added. The mixture was stirred and refluxed for 24 h. Then solids were filtered off and solvent was removed. The residue was washed with toluene (3x10 mL) and dissolved in boiling acetonitrile (10 mL). The resulting acetonitrile solution was kept in fridge to give yellow crystals of **3b**, which were collected by filtration. A single crystal for X-ray analysis was grown on slow cooling of acetonitrile solution. Yield 46% (55 mg, 0.07 mmol). ^{1}H NMR ($CDCl_3$), δ: 9.26 (1H, dd, ^{3}J = 5.0, ^{4}J = 1.0 Hz, H6′), 8.39 (1H, d, ^{3}J = 8.0 Hz, H3′), 8.31 (2H, m, H4′+H4), 8.04 (1H, ^{3}J = 8.0 Hz, H3), 7.91 (1H, dd, $^{3}J_1$ = 8.0, $^{3}J_2$ = 5.0, Hz, H5′), 7.66 (2H, m, Ar), 7.40-7.26 (6H, m, Ar), 7.16 (1H, m, Ar), 1.83 (3H, s, Me), 3.40-1.60 (9H, br.m, B-H). ^{11}B{^{1}H} NMR ($CDCl_3$), δ: –0.3 (2B), –2.9 (2B), –5.5 (1B), –7.9 (2B), –9.5 (1B), –12.2 (1B). ESI-MS, m/z: found 763.1954, calcd. 763.1936 for $C_{27}H_{27}B_{10}BrN_2Pt$.

Computational methods

For all calculations, the *Orca 2.8.0* package of programs was used.[2] In the RKS-DFT calculations

[2] "Orca 2.8.0. " – calculation program package. F. Neese *et al.*, Universitaet Bonn, Bonn, Germany,2010.

the B3LYP hybrid functional was applied.[3,4] The metals were described by the Stuttgart-Dresden[5] effective core potential (treating the valence electrons explicitly) using the Ahlrichs def2-TZVP[6] basis set of triple-ζ quality together with the Ahlrichs auxiliary basis set (def2-TZVP/J)[7], while the Ahlrichs triple-ζ basis set TZVP[8] and TZVP/J auxiliary basis were used for non-metal atoms. The COSMO solvation model[9] was used to calculate solvent effect in DCM (ε = 9.08, n_D = 1.424). The ground state geometries of the complexes were fully optimized without symmetry constraints. To accelerate calculations we employed the RIJCOSX approximation combining RI-J method and COSX approximation. It means, that in performing two electron integrals, the first integration is done numerically on a grid and the second (involving the Coulomb singularity) is done analytically.[10]

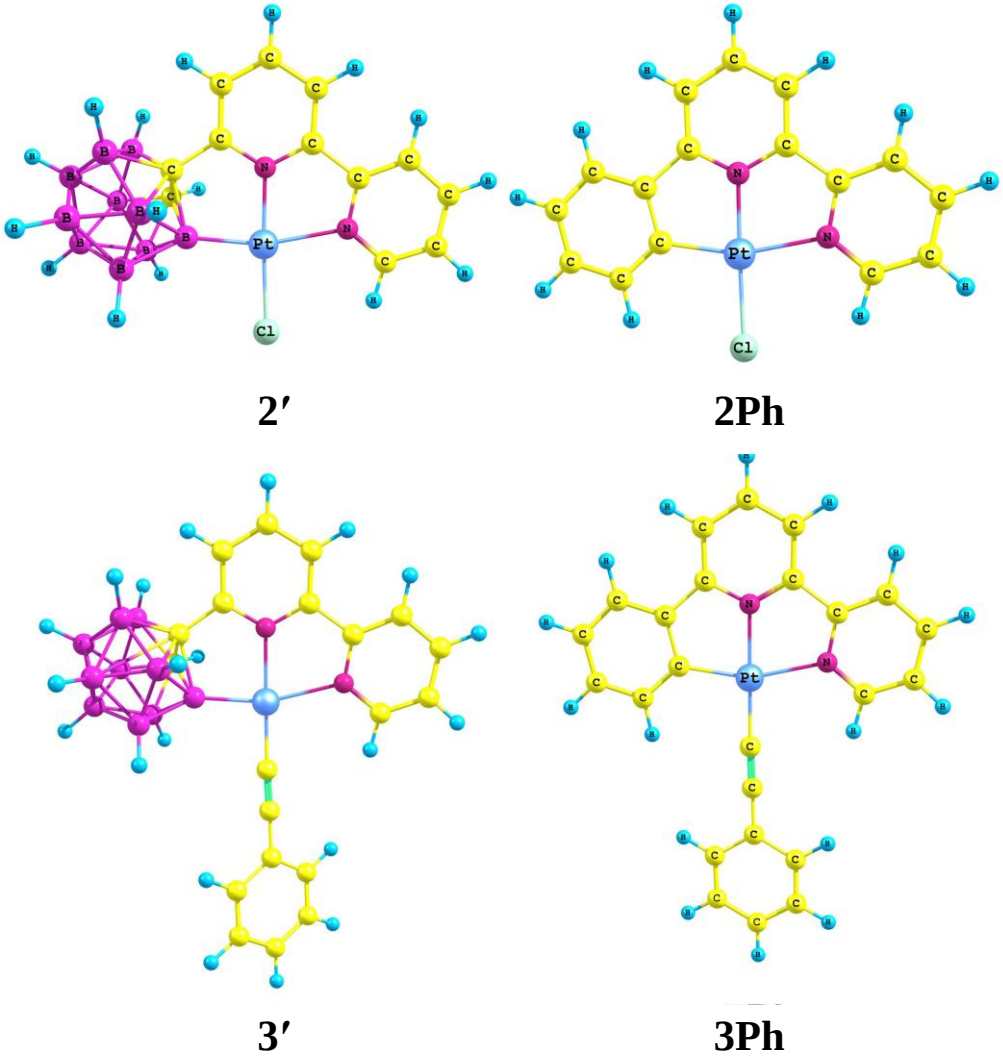


Figure S1. Calculated geometries of the Pt complexes

3 A.D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.

4 C. Lee, W. Yang and R.G. Parr, *Phys. Rev. B* **1988**, *37*, 785.

5 D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990,** *77*, 123.

6 F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

7 F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057.

8 A. Schaefer, H. Horn, R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571.

9 A. Klamt, G. Schüürmann, *J. Chem. Soc., Perkin Trans.* 2, **1993**, 799.

10 F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, *356*, 98.

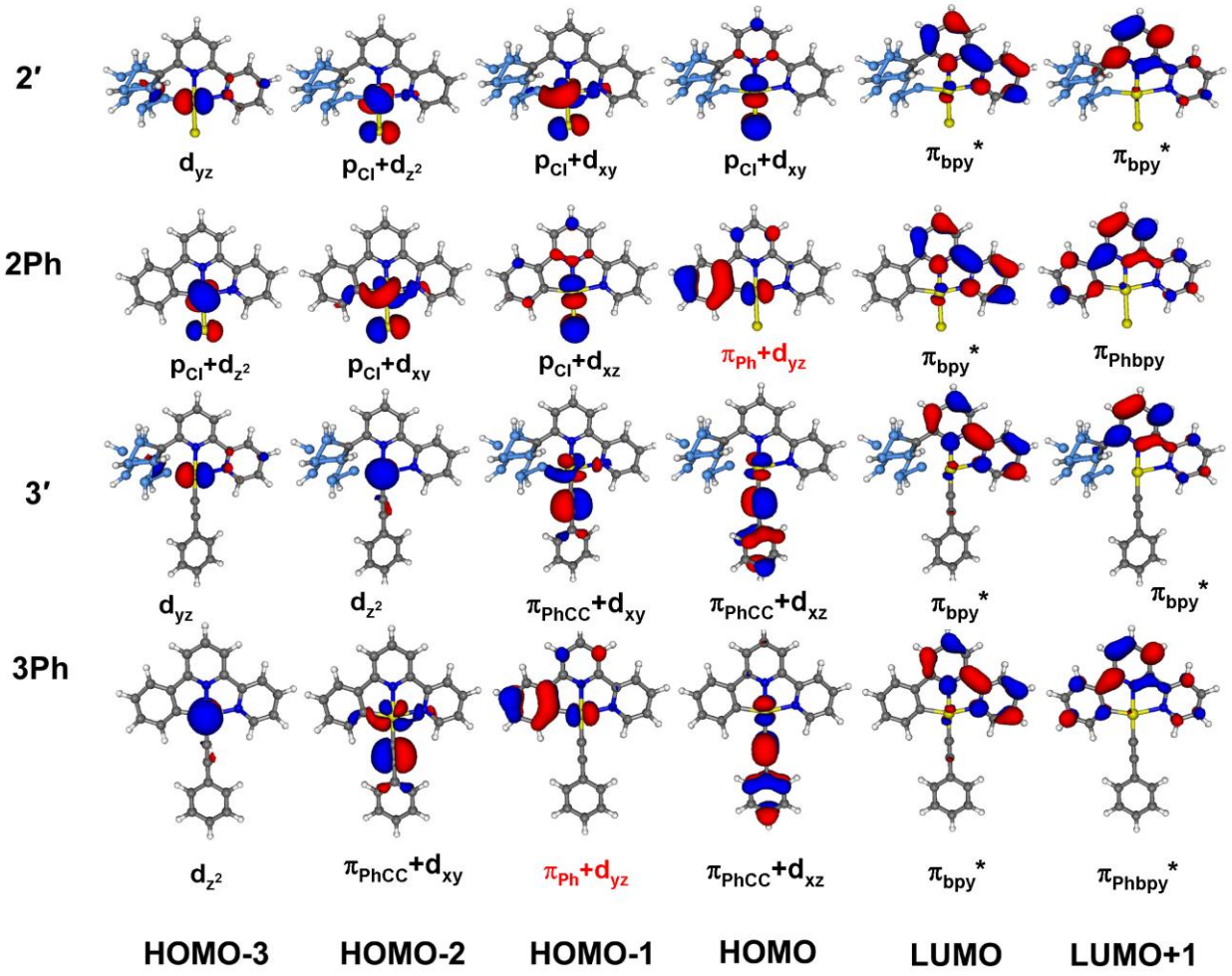


Figure S2. Contour plots of the frontier molecular orbitals in the ground state of the Pt complexes.

Crystallographic Data

X-ray structures were determined using a Oxford Diffraction Xcalibur S system (MoK_α radiation, λ = 0.71093 Å, graphite monochromator, $\omega/2\theta$ scan). Analytical absorptions correction was performed.[11] Structure solution and structure refinement was performed using *SHELXL-97* program package.[12,13] Nonhydrogen atoms were refined by full-matrix least-squares procedures (with F^2) in an anisotropic approximation. H-atoms were added in calculated positions and refined in an isotropic approximation in the "riding" model.

Crystallographic data (excluding structure factors) for structure in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 817579 & 817580. Copies of the data can be obtained free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 (0) 1223 336033 or e-mail: deposit@ccdc.cam.ac.uk). Abbreviated crystallographic data are given in Table S1.

Table S1. Crystal data and structure refinement

11 Clark, R. C., Reid, J. S *Acta Crystallogr., Sect. A: Found. Crystallogr.* **1995**, *51*, 887.

12 Sheldrick G. M., *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112.

13 "SHELXL-97" - program for the Refinement of Crystal Structures. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, 1997.

	2a	**3b**
Crystal size, mm	0.12x0.08x0.04	0.15x0.11x0.05
Crystal color	orange	orange
Empirical formula	$C_{25}H_{27}B_{10}ClN_2Pt$	$C_{27}H_{27}B_{10}BrN_2Pt$
Formula weight	694.13	762.61
Temperature, K	295(2)	295(2)
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1/n$	Pbca
a, Å	10.7374(7)	17.4108(4)
b, Å	15.9467(10)	16.0201(9)
c, Å	16.1973(12)	21.0923(12)
α, °	90	90
β, °	92.138(5)	90
γ, °	90	90
Volume, Z	2771.5(3) Å^3, 4	5883.1(5) Å^3, 8
μ, mm^{-1}	5.180	6.151
D_{calc}, g/cm^3	1.664	1.722
θ range for data collection, °	2.65 to 28.30°	2.72 to 26.39
Reflections collected	11046	22833
Independent reflections(R_{int})	6469 (0.0510)	5997(0.0449)
Reflections with I>2σ(I)	3156	3178
Completeness (to θ, °)	96.5 % (26.00)	99.5 % (26.39)
S	0.996	1.006
R_1 [I>2σ(I)]	0.0393	0.0255
wR_2 [I>2σ(I)]	0.0540	0.0359
R_1 (all data)	0.1099	0.0689
wR_2 (all data)	0.0698	0.0373
Largest diff. peak and hole, ē/Å^3	1.343/-1.392	1.134/-0.546

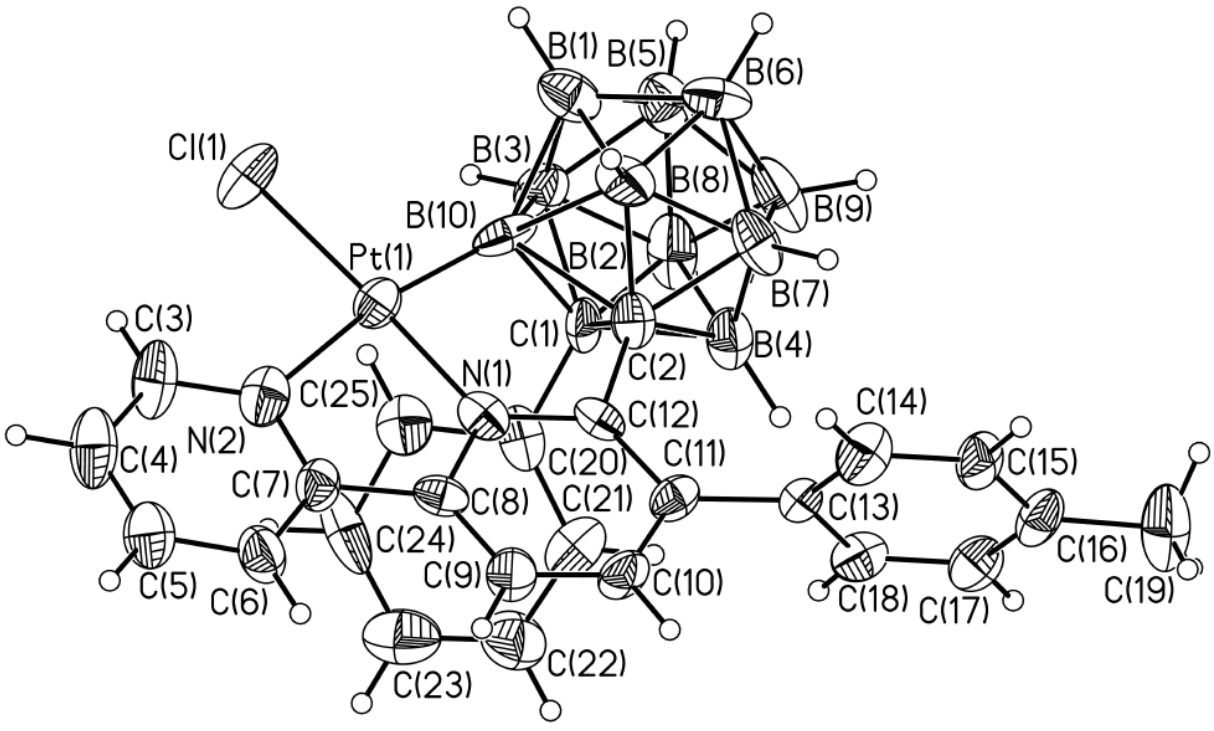


Figure S3. Molecular structure of **2a**

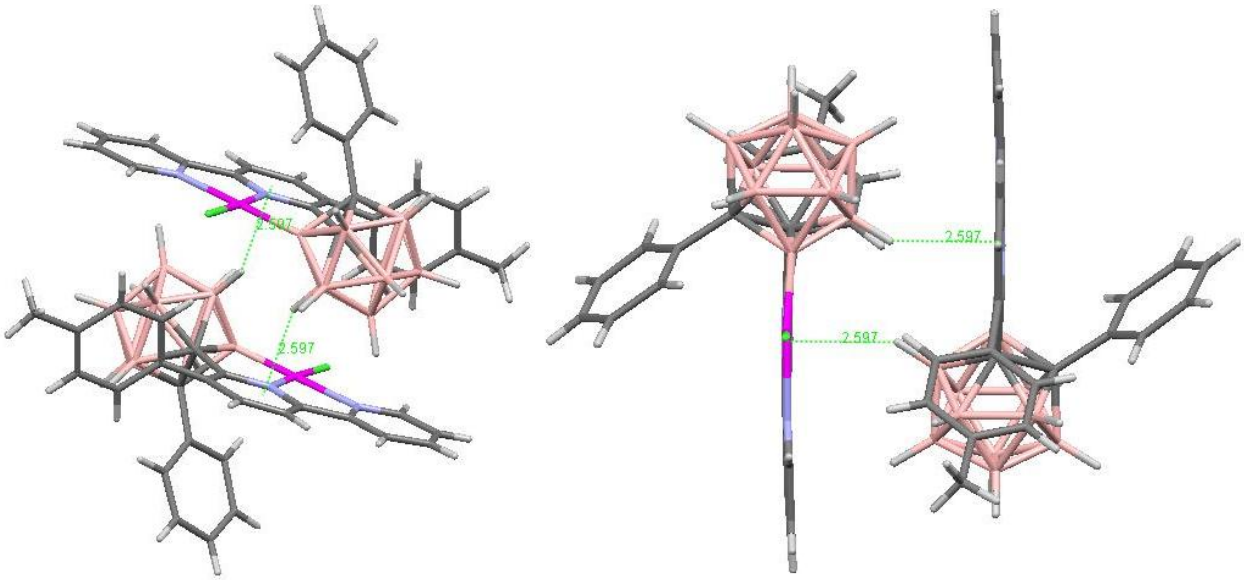


Figure S4. Crystal packing of **2a**

Table S2. Bond lengths [A] and angles [deg] for **2a**

Pt1	**B10**	1.903(9)	**B3**	**B5**	1.767(12)
Pt1	**N1**	1.951(6)	**B3**	**B10**	1.814(12)
Pt1	**N2**	2.118(6)	**B3**	**H3**	1.1000
Pt1	**Cl1**	2.284(2)	**B10**	**B8**	1.805(11)
N1	**C12**	1.384(8)	**C4**	**C5**	1.380(10)
N1	**C8**	1.386(7)	**C4**	**H4A**	0.9300
C1	**C20**	1.572(9)	**C5**	**C6**	1.354(10)
C1	**C2**	1.685(9)	**C5**	**H5A**	0.9300
C1	**B2**	1.715(10)	**B5**	**B6**	1.748(13)
C1	**B3**	1.724(11)	**B5**	**B9**	1.766(15)
C1	**B4**	1.735(11)	**B5**	**H5**	1.1000
C1	**B10**	1.841(12)	**C6**	**C7**	1.371(9)
B1	**B8**	1.742(13)	**C6**	**H6A**	0.9300
B1	**B6**	1.745(13)	**B6**	**B8**	1.734(11)
B1	**B5**	1.758(13)	**B6**	**B9**	1.778(15)
B1	**B3**	1.773(12)	**B6**	**B7**	1.805(13)
B1	**B10**	1.826(11)	**B6**	**H6**	1.1000
B1	**H1**	1.1000	**C7**	**C8**	1.470(9)
N2	**C3**	1.318(9)	**B7**	**B8**	1.769(12)
N2	**C7**	1.374(8)	**B7**	**B9**	1.768(12)
C2	**C12**	1.536(8)	**B7**	**B4**	1.783(12)
C2	**B7**	1.709(9)	**B7**	**H7**	1.1000
C2	**B8**	1.725(10)	**B8**	**H8**	1.1000
C2	**B4**	1.727(11)	**C8**	**C9**	1.361(9)
C2	**B10**	1.843(11)	**C9**	**C10**	1.342(9)
B2	**B9**	1.756(12)	**C9**	**H9A**	0.9300
B2	**B3**	1.784(13)	**B9**	**B4**	1.803(13)
B2	**B4**	1.821(12)	**B9**	**H9**	1.1000
B2	**B5**	1.821(14)	**C10**	**C11**	1.387(8)
B2	**H2**	1.1000	**C10**	**H10A**	0.9300
C3	**C4**	1.397(9)	**B4**	**H4**	1.1000
C3	**H3A**	0.9300	**C11**	**C12**	1.402(9)

C11	**C13**	1.479(9)
C13	**C18**	1.391(9)
C13	**C14**	1.399(8)
C14	**C15**	1.353(9)
C14	**H14A**	0.9300
C15	**C16**	1.416(10)
C15	**H15A**	0.9300
C16	**C17**	1.371(9)
C16	**C19**	1.476(10)
C17	**C18**	1.362(9)
C17	**H17A**	0.9300
C18	**H18A**	0.9300
C19	**H19A**	0.9600

C19	**H19B**	0.9600
C19	**H19C**	0.9600
C20	**C25**	1.407(10)
C20	**C21**	1.428(11)
C21	**C22**	1.348(10)
C21	**H21A**	0.9300
C22	**C23**	1.324(11)
C22	**H22A**	0.9300
C23	**C24**	1.392(12)
C23	**H23A**	0.9300
C24	**C25**	1.462(9)
C24	**H24A**	0.9300
C25	**H25A**	0.9300

B10	**Pt1**	**N1**	87.6(3)
B10	**Pt1**	**N2**	167.0(3)
N1	**Pt1**	**N2**	80.0(2)
B10	**Pt1**	**Cl1**	94.3(3)
N1	**Pt1**	**Cl1**	177.80(16)
N2	**Pt1**	**Cl1**	98.15(19)
C12	**N1**	**C8**	117.9(6)
C12	**N1**	**Pt1**	124.1(4)
C8	**N1**	**Pt1**	118.0(5)
C20	**C1**	**C2**	117.0(5)
C20	**C1**	**B2**	121.5(6)
C2	**C1**	**B2**	111.1(5)
C20	**C1**	**B3**	123.7(6)
C2	**C1**	**B3**	109.6(6)
B2	**C1**	**B3**	62.5(5)
C20	**C1**	**B4**	115.2(7)
C2	**C1**	**B4**	60.6(4)
B2	**C1**	**B4**	63.7(5)
B3	**C1**	**B4**	114.3(6)
C20	**C1**	**B10**	115.8(6)
C2	**C1**	**B10**	62.9(4)
B2	**C1**	**B10**	114.7(6)
B3	**C1**	**B10**	61.1(5)
B4	**C1**	**B10**	115.8(5)
B8	**B1**	**B6**	59.6(5)
B8	**B1**	**B5**	106.9(7)
B6	**B1**	**B5**	59.9(5)
B8	**B1**	**B3**	105.6(7)
B6	**B1**	**B3**	107.1(8)
B5	**B1**	**B3**	60.1(5)
B8	**B1**	**B10**	60.7(4)
B6	**B1**	**B10**	110.8(7)
B5	**B1**	**B10**	110.9(7)
B3	**B1**	**B10**	60.5(4)
B8	**B1**	**H1**	123.3
B6	**B1**	**H1**	121.3
B5	**B1**	**H1**	121.2
B3	**B1**	**H1**	123.1

B10	**B1**	**H1**	119.0
C3	**N2**	**C7**	118.3(7)
C3	**N2**	**Pt1**	128.8(6)
C7	**N2**	**Pt1**	112.9(5)
C12	**C2**	**C1**	117.6(5)
C12	**C2**	**B7**	126.6(6)
C1	**C2**	**B7**	109.7(5)
C12	**C2**	**B8**	119.8(6)
C1	**C2**	**B8**	108.1(6)
B7	**C2**	**B8**	62.0(5)
C12	**C2**	**B4**	122.4(6)
C1	**C2**	**B4**	61.1(4)
B7	**C2**	**B4**	62.5(5)
B8	**C2**	**B4**	112.9(5)
C12	**C2**	**B10**	108.9(5)
C1	**C2**	**B10**	62.7(4)
B7	**C2**	**B10**	113.9(6)
B8	**C2**	**B10**	60.7(4)
B4	**C2**	**B10**	116.1(5)
C1	**B2**	**B9**	104.5(6)
C1	**B2**	**B3**	59.0(5)
B9	**B2**	**B3**	105.5(8)
C1	**B2**	**B4**	58.7(4)
B9	**B2**	**B4**	60.5(5)
B3	**B2**	**B4**	107.5(6)
C1	**B2**	**B5**	104.7(7)
B9	**B2**	**B5**	59.1(6)
B3	**B2**	**B5**	58.7(5)
B4	**B2**	**B5**	108.2(7)
C1	**B2**	**H2**	124.4
B9	**B2**	**H2**	123.3
B3	**B2**	**H2**	122.8
B4	**B2**	**H2**	121.1
B5	**B2**	**H2**	122.7
N2	**C3**	**C4**	121.2(8)
N2	**C3**	**H3A**	119.4
C4	**C3**	**H3A**	119.4
C1	**B3**	**B5**	106.7(7)

C1	**B3**	**B1**	107.6(6)
B5	**B3**	**B1**	59.6(5)
C1	**B3**	**B2**	58.5(5)
B5	**B3**	**B2**	61.7(5)
B1	**B3**	**B2**	109.7(7)
C1	**B3**	**B10**	62.6(4)
B5	**B3**	**B10**	111.1(6)
B1	**B3**	**B10**	61.2(5)
B2	**B3**	**B10**	112.6(6)
C1	**B3**	**H3**	123.0
B5	**B3**	**H3**	121.4
B1	**B3**	**H3**	121.8
B2	**B3**	**H3**	119.9
B10	**B3**	**H3**	117.9
B8	**B10**	**B3**	101.3(6)
B8	**B10**	**B1**	57.3(5)
B3	**B10**	**B1**	58.3(4)
B8	**B10**	**C2**	56.4(4)
B3	**B10**	**C2**	99.2(6)
B1	**B10**	**C2**	100.7(6)
B8	**B10**	**C1**	98.5(6)
B3	**B10**	**C1**	56.3(4)
B1	**B10**	**C1**	100.6(6)
C2	**B10**	**C1**	54.4(4)
B8	**B10**	**Pt1**	121.0(5)
B3	**B10**	**Pt1**	137.3(5)
B1	**B10**	**Pt1**	141.2(6)
C2	**B10**	**Pt1**	108.3(4)
C1	**B10**	**Pt1**	117.1(5)
C5	**C4**	**C3**	119.6(8)
C5	**C4**	**H4A**	120.2
C3	**C4**	**H4A**	120.2
C6	**C5**	**C4**	119.5(8)
C6	**C5**	**H5A**	120.2
C4	**C5**	**H5A**	120.2
B6	**B5**	**B1**	59.7(5)
B6	**B5**	**B9**	60.8(5)
B1	**B5**	**B9**	108.0(7)
B6	**B5**	**B3**	107.3(6)
B1	**B5**	**B3**	60.4(5)
B9	**B5**	**B3**	105.8(7)
B6	**B5**	**B2**	108.0(7)
B1	**B5**	**B2**	108.7(6)
B9	**B5**	**B2**	58.6(5)
B3	**B5**	**B2**	59.6(5)
B6	**B5**	**H5**	121.6
B1	**B5**	**H5**	121.1
B9	**B5**	**H5**	122.6
B3	**B5**	**H5**	122.7
B2	**B5**	**H5**	121.8
C5	**C6**	**C7**	118.8(8)
C5	**C6**	**H6A**	120.6
C7	**C6**	**H6A**	120.6
B8	**B6**	**B1**	60.1(5)
B8	**B6**	**B5**	107.7(6)
B1	**B6**	**B5**	60.4(5)
B8	**B6**	**B9**	106.3(6)
B1	**B6**	**B9**	108.1(7)
B5	**B6**	**B9**	60.1(5)
B8	**B6**	**B7**	60.0(5)
B1	**B6**	**B7**	108.9(6)
B5	**B6**	**B7**	108.3(7)
B9	**B6**	**B7**	59.1(5)
B8	**B6**	**H6**	122.5
B1	**B6**	**H6**	121.0
B5	**B6**	**H6**	121.4
B9	**B6**	**H6**	122.6
B7	**B6**	**H6**	121.5
C6	**C7**	**N2**	122.6(7)
C6	**C7**	**C8**	122.8(7)
N2	**C7**	**C8**	114.5(7)
C2	**B7**	**B8**	59.4(4)
C2	**B7**	**B9**	105.2(6)
B8	**B7**	**B9**	105.2(7)
C2	**B7**	**B4**	59.2(4)
B8	**B7**	**B4**	108.2(6)
B9	**B7**	**B4**	61.0(5)
C2	**B7**	**B6**	105.4(6)
B8	**B7**	**B6**	58.1(5)
B9	**B7**	**B6**	59.7(6)
B4	**B7**	**B6**	109.6(6)
C2	**B7**	**H7**	123.8
B8	**B7**	**H7**	123.0
B9	**B7**	**H7**	123.1
B4	**B7**	**H7**	120.2
B6	**B7**	**H7**	122.3
C2	**B8**	**B6**	107.8(6)
C2	**B8**	**B1**	109.1(6)
B6	**B8**	**B1**	60.3(5)
C2	**B8**	**B7**	58.6(4)
B6	**B8**	**B7**	62.0(5)
B1	**B8**	**B7**	110.7(7)
C2	**B8**	**B10**	62.9(4)
B6	**B8**	**B10**	112.3(7)
B1	**B8**	**B10**	61.9(5)
B7	**B8**	**B10**	112.9(6)
C2	**B8**	**H8**	122.3
B6	**B8**	**H8**	120.6
B1	**B8**	**H8**	120.8
B7	**B8**	**H8**	119.8
B10	**B8**	**H8**	117.4
C9	**C8**	**N1**	120.8(7)
C9	**C8**	**C7**	124.5(7)
N1	**C8**	**C7**	114.7(7)

C10	**C9**	**C8**	119.7(7)
C10	**C9**	**H9A**	120.1
C8	**C9**	**H9A**	120.1
B2	**B9**	**B5**	62.2(6)
B2	**B9**	**B7**	109.5(6)
B5	**B9**	**B7**	109.1(8)
B2	**B9**	**B6**	109.6(8)
B5	**B9**	**B6**	59.1(6)
B7	**B9**	**B6**	61.2(5)
B2	**B9**	**B4**	61.5(5)
B5	**B9**	**B4**	111.4(7)
B7	**B9**	**B4**	59.9(5)
B6	**B9**	**B4**	109.8(7)
B2	**B9**	**H9**	120.0
B5	**B9**	**H9**	120.4
B7	**B9**	**H9**	121.3
B6	**B9**	**H9**	121.3
B4	**B9**	**H9**	120.0
C9	**C10**	**C11**	123.8(7)
C9	**C10**	**H10A**	118.1
C11	**C10**	**H10A**	118.1
C2	**B4**	**C1**	58.3(4)
C2	**B4**	**B7**	58.3(5)
C1	**B4**	**B7**	104.2(7)
C2	**B4**	**B9**	103.0(7)
C1	**B4**	**B9**	101.7(7)
B7	**B4**	**B9**	59.1(5)
C2	**B4**	**B2**	104.3(7)
C1	**B4**	**B2**	57.6(4)
B7	**B4**	**B2**	106.0(7)
B9	**B4**	**B2**	58.0(5)
C2	**B4**	**H4**	124.3
C1	**B4**	**H4**	125.1
B7	**B4**	**H4**	122.8
B9	**B4**	**H4**	125.2
B2	**B4**	**H4**	123.4
C10	**C11**	**C12**	115.0(7)
C10	**C11**	**C13**	118.1(7)
C12	**C11**	**C13**	126.6(6)
N1	**C12**	**C11**	122.7(6)
N1	**C12**	**C2**	111.1(6)
C11	**C12**	**C2**	126.1(7)
C18	**C13**	**C14**	118.4(7)
C18	**C13**	**C11**	124.2(7)
C14	**C13**	**C11**	117.0(7)
C15	**C14**	**C13**	120.0(8)
C15	**C14**	**H14A**	120.0
C13	**C14**	**H14A**	120.0
C14	**C15**	**C16**	121.7(7)
C14	**C15**	**H15A**	119.1
C16	**C15**	**H15A**	119.1
C17	**C16**	**C15**	117.2(7)
C17	**C16**	**C19**	122.3(8)
C15	**C16**	**C19**	120.5(7)
C18	**C17**	**C16**	121.7(8)
C18	**C17**	**H17A**	119.1
C16	**C17**	**H17A**	119.1
C17	**C18**	**C13**	120.9(7)
C17	**C18**	**H18A**	119.6
C13	**C18**	**H18A**	119.6
C16	**C19**	**H19A**	109.5
C16	**C19**	**H19B**	109.5
H19A	**C19**	**H19B**	109.5
C16	**C19**	**H19C**	109.5
H19A	**C19**	**H19C**	109.5
H19B	**C19**	**H19C**	109.5
C25	**C20**	**C21**	120.4(7)
C25	**C20**	**C1**	114.6(8)
C21	**C20**	**C1**	124.9(7)
C22	**C21**	**C20**	120.2(8)
C22	**C21**	**H21A**	119.9
C20	**C21**	**H21A**	119.9
C23	**C22**	**C21**	123.4(10)
C23	**C22**	**H22A**	118.3
C21	**C22**	**H22A**	118.3
C22	**C23**	**C24**	118.7(9)
C22	**C23**	**H23A**	120.6
C24	**C23**	**H23A**	120.6
C23	**C24**	**C25**	122.8(8)
C23	**C24**	**H24A**	118.6
C25	**C24**	**H24A**	118.6
C20	**C25**	**C24**	114.4(8)
C20	**C25**	**H25A**	122.8
C24	**C25**	**H25A**	122.8

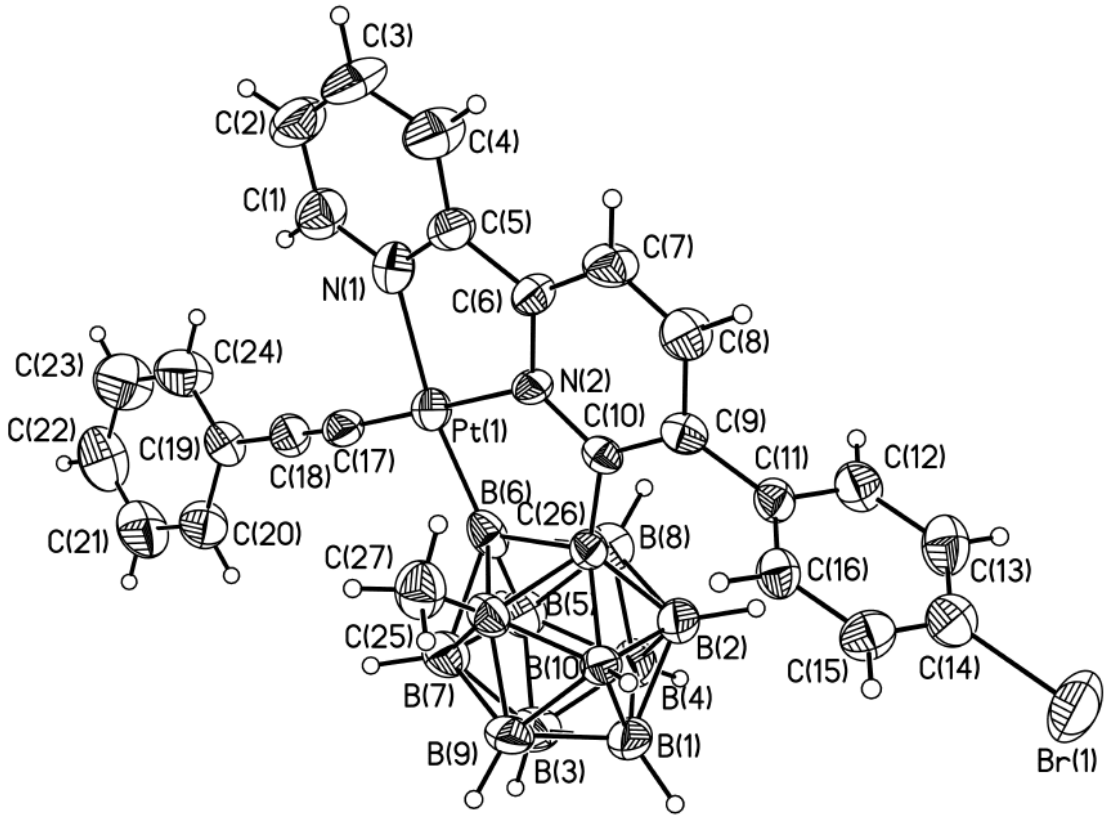


Figure S5. Molecular structure of **3b**

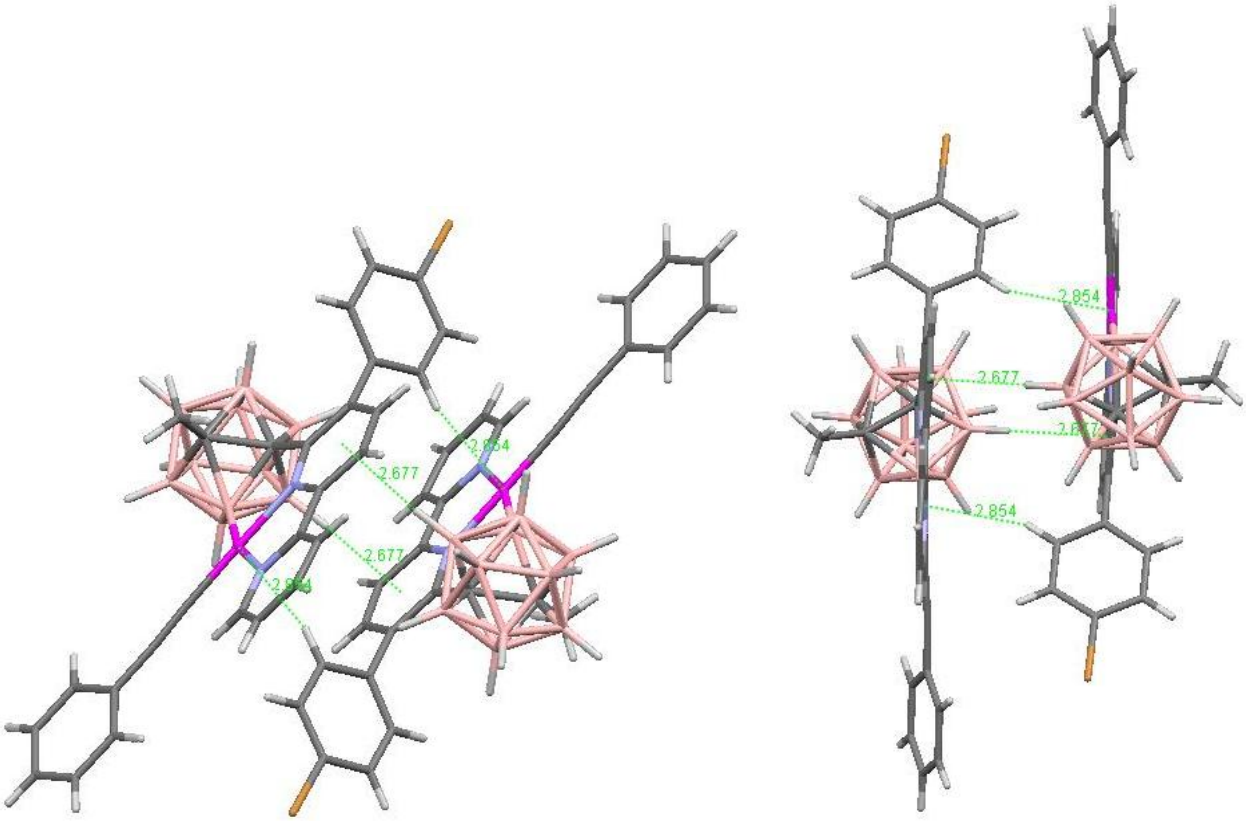


Figure S6. Crystal packing of **3b**

Table S3. Bond lengths [A] and angles [deg] for **3b**

Pt1	**C17**	1.925(4)
Pt1	**B6**	1.941(5)
Pt1	**N2**	2.022(3)
Pt1	**N1**	2.122(4)
Br1	**C14**	1.882(5)
N1	**C1**	1.338(5)
N1	**C5**	1.366(5)
C1	**C2**	1.377(6)
C1	**H1A**	0.9300
B1	**B10**	1.747(7)
B1	**B9**	1.762(7)
B1	**B2**	1.769(7)
B1	**B3**	1.778(7)
B1	**B4**	1.778(8)
B1	**H1**	1.1000
N2	**C10**	1.353(5)
N2	**C6**	1.354(5)
B2	**C26**	1.698(6)
B2	**B8**	1.748(7)
B2	**B10**	1.761(7)
B2	**B4**	1.763(7)
B2	**H2**	1.1000
C2	**C3**	1.369(5)
C2	**H2A**	0.9300
C3	**C4**	1.381(6)
C3	**H3A**	0.9300
B3	**B7**	1.756(7)
B3	**B9**	1.756(8)
B3	**B4**	1.763(7)
B3	**B5**	1.773(7)
B3	**H3**	1.1000
B4	**B8**	1.776(7)
B4	**B5**	1.787(7)
B4	**H4**	1.1000
C4	**C5**	1.391(6)
C4	**H4A**	0.9300
C5	**C6**	1.473(6)
B5	**B7**	1.745(7)
B5	**B8**	1.782(6)
B5	**B6**	1.802(7)
B5	**H5**	1.1000
B6	**B7**	1.800(6)
B6	**C25**	1.806(5)
B6	**C26**	1.831(5)
B6	**B8**	1.836(7)
C6	**C7**	1.386(5)
B7	**C25**	1.705(6)
B7	**B9**	1.795(7)
B7	**H7**	1.1000
C7	**C8**	1.360(6)
C7	**H7A**	0.9300
C8	**C9**	1.406(5)
C8	**H8A**	0.9300
B8	**C26**	1.686(6)
B8	**H8**	1.1000
B9	**C25**	1.705(6)
B9	**B10**	1.753(6)
B9	**H9**	1.1000
C9	**C10**	1.411(5)
C9	**C11**	1.488(5)
C10	**C26**	1.510(5)
B10	**C26**	1.709(6)
B10	**C25**	1.714(6)
B10	**H10**	1.1000
C11	**C12**	1.373(5)
C11	**C16**	1.400(5)
C12	**C13**	1.384(6)
C12	**H12A**	0.9300
C13	**C14**	1.389(6)
C13	**H13A**	0.9300
C14	**C15**	1.380(5)
C15	**C16**	1.371(5)
C15	**H15A**	0.9300
C16	**H16A**	0.9300
C17	**C18**	1.218(5)
C18	**C19**	1.443(5)
C19	**C24**	1.356(6)
C19	**C20**	1.390(5)
C20	**C21**	1.378(5)
C20	**H20A**	0.9300
C21	**C22**	1.357(7)
C21	**H21A**	0.9300
C22	**C23**	1.347(6)
C22	**H22A**	0.9300
C23	**C24**	1.383(6)
C23	**H23A**	0.9300
C24	**H24A**	0.9300
C25	**C27**	1.499(5)
C25	**C26**	1.660(5)
C27	**H27A**	0.9600
C27	**H27B**	0.9600
C27	**H27C**	0.9600

C17	**Pt1**	**B6**	94.64(17)
C17	**Pt1**	**N2**	178.84(14)

B6	**Pt1**	**N2**	85.59(15)
C17	**Pt1**	**N1**	100.24(16)
B6	**Pt1**	**N1**	165.08(15)
N2	**Pt1**	**N1**	79.56(14)
C1	**N1**	**C5**	117.7(4)
C1	**N1**	**Pt1**	129.3(3)
C5	**N1**	**Pt1**	112.8(3)
N1	**C1**	**C2**	124.0(4)
N1	**C1**	**H1A**	118.0
C2	**C1**	**H1A**	118.0
B10	**B1**	**B9**	59.9(3)
B10	**B1**	**B2**	60.1(3)
B9	**B1**	**B2**	107.7(4)
B10	**B1**	**B3**	107.0(4)
B9	**B1**	**B3**	59.5(3)
B2	**B1**	**B3**	106.7(4)
B10	**B1**	**B4**	107.6(4)
B9	**B1**	**B4**	107.5(4)
B2	**B1**	**B4**	59.6(3)
B3	**B1**	**B4**	59.5(3)
B10	**B1**	**H1**	121.9
B9	**B1**	**H1**	121.9
B2	**B1**	**H1**	122.1
B3	**B1**	**H1**	122.7
B4	**B1**	**H1**	122.1
C10	**N2**	**C6**	121.3(3)
C10	**N2**	**Pt1**	122.6(3)
C6	**N2**	**Pt1**	116.0(3)
C26	**B2**	**B8**	58.6(3)
C26	**B2**	**B10**	59.2(3)
B8	**B2**	**B10**	107.8(3)
C26	**B2**	**B4**	105.8(4)
B8	**B2**	**B4**	60.8(3)
B10	**B2**	**B4**	107.7(3)
C26	**B2**	**B1**	105.6(4)
B8	**B2**	**B1**	108.9(4)
B10	**B2**	**B1**	59.3(3)
B4	**B2**	**B1**	60.4(3)
C26	**B2**	**H2**	124.1
B8	**B2**	**H2**	121.2
B10	**B2**	**H2**	122.0
B4	**B2**	**H2**	121.8
B1	**B2**	**H2**	121.9
C3	**C2**	**C1**	117.5(5)
C3	**C2**	**H2A**	121.2
C1	**C2**	**H2A**	121.2
C2	**C3**	**C4**	120.9(5)
C2	**C3**	**H3A**	119.5
C4	**C3**	**H3A**	119.5
B7	**B3**	**B9**	61.5(3)
B7	**B3**	**B4**	108.2(4)
B9	**B3**	**B4**	108.4(4)

B7	**B3**	**B5**	59.3(3)
B9	**B3**	**B5**	109.0(4)
B4	**B3**	**B5**	60.7(3)
B7	**B3**	**B1**	109.0(4)
B9	**B3**	**B1**	59.8(3)
B4	**B3**	**B1**	60.3(3)
B5	**B3**	**B1**	109.1(4)
B7	**B3**	**H3**	121.3
B9	**B3**	**H3**	121.1
B4	**B3**	**H3**	121.5
B5	**B3**	**H3**	121.3
B1	**B3**	**H3**	121.2
B2	**B4**	**B3**	107.7(4)
B2	**B4**	**B8**	59.2(3)
B3	**B4**	**B8**	107.2(4)
B2	**B4**	**B1**	60.0(3)
B3	**B4**	**B1**	60.3(3)
B8	**B4**	**B1**	107.3(4)
B2	**B4**	**B5**	107.7(4)
B3	**B4**	**B5**	59.9(3)
B8	**B4**	**B5**	60.0(3)
B1	**B4**	**B5**	108.4(4)
B2	**B4**	**H4**	122.1
B3	**B4**	**H4**	121.9
B8	**B4**	**H4**	122.5
B1	**B4**	**H4**	121.6
B5	**B4**	**H4**	121.5
C3	**C4**	**C5**	118.4(5)
C3	**C4**	**H4A**	120.8
C5	**C4**	**H4A**	120.8
N1	**C5**	**C4**	121.4(4)
N1	**C5**	**C6**	115.1(4)
C4	**C5**	**C6**	123.4(4)
B7	**B5**	**B3**	59.9(3)
B7	**B5**	**B8**	107.1(3)
B3	**B5**	**B8**	106.6(4)
B7	**B5**	**B4**	107.6(4)
B3	**B5**	**B4**	59.4(3)
B8	**B5**	**B4**	59.7(3)
B7	**B5**	**B6**	61.0(3)
B3	**B5**	**B6**	110.6(3)
B8	**B5**	**B6**	61.6(3)
B4	**B5**	**B6**	111.4(3)
B7	**B5**	**H5**	122.3
B3	**B5**	**H5**	121.9
B8	**B5**	**H5**	122.6
B4	**B5**	**H5**	121.2
B6	**B5**	**H5**	118.6
B7	**B6**	**B5**	58.0(3)
B7	**B6**	**C25**	56.4(2)
B5	**B6**	**C25**	99.7(3)
B7	**B6**	**C26**	99.1(3)

B5	**B6**	**C26**	99.4(3)
C25	**B6**	**C26**	54.3(2)
B7	**B6**	**B8**	102.6(4)
B5	**B6**	**B8**	58.6(3)
C25	**B6**	**B8**	97.8(3)
C26	**B6**	**B8**	54.8(2)
B7	**B6**	**Pt1**	136.1(3)
B5	**B6**	**Pt1**	142.4(3)
C25	**B6**	**Pt1**	116.6(3)
C26	**B6**	**Pt1**	109.1(3)
B8	**B6**	**Pt1**	121.0(3)
N2	**C6**	**C7**	120.3(4)
N2	**C6**	**C5**	116.1(4)
C7	**C6**	**C5**	123.6(4)
C25	**B7**	**B5**	106.1(3)
C25	**B7**	**B3**	104.5(4)
B5	**B7**	**B3**	60.8(3)
C25	**B7**	**B9**	58.2(3)
B5	**B7**	**B9**	108.5(4)
B3	**B7**	**B9**	59.3(3)
C25	**B7**	**B6**	62.0(2)
B5	**B7**	**B6**	61.1(3)
B3	**B7**	**B6**	111.4(4)
B9	**B7**	**B6**	111.8(3)
C25	**B7**	**H7**	124.3
B5	**B7**	**H7**	121.9
B3	**B7**	**H7**	122.0
B9	**B7**	**H7**	121.2
B6	**B7**	**H7**	117.8
C8	**C7**	**C6**	118.9(4)
C8	**C7**	**H7A**	120.5
C6	**C7**	**H7A**	120.5
C7	**C8**	**C9**	122.5(4)
C7	**C8**	**H8A**	118.8
C9	**C8**	**H8A**	118.8
C26	**B8**	**B2**	59.2(3)
C26	**B8**	**B4**	105.7(4)
B2	**B8**	**B4**	60.0(3)
C26	**B8**	**B5**	106.1(3)
B2	**B8**	**B5**	108.7(4)
B4	**B8**	**B5**	60.3(3)
C26	**B8**	**B6**	62.5(2)
B2	**B8**	**B6**	112.6(3)
B4	**B8**	**B6**	110.3(3)
B5	**B8**	**B6**	59.7(3)
C26	**B8**	**H8**	123.3
B2	**B8**	**H8**	120.2
B4	**B8**	**H8**	122.0
B5	**B8**	**H8**	122.7
B6	**B8**	**H8**	118.4
C25	**B9**	**B10**	59.4(3)
C25	**B9**	**B3**	104.4(4)

B10	**B9**	**B3**	107.7(4)
C25	**B9**	**B1**	105.6(3)
B10	**B9**	**B1**	59.6(3)
B3	**B9**	**B1**	60.7(3)
C25	**B9**	**B7**	58.2(3)
B10	**B9**	**B7**	107.5(4)
B3	**B9**	**B7**	59.3(3)
B1	**B9**	**B7**	108.0(4)
C25	**B9**	**H9**	124.4
B10	**B9**	**H9**	121.7
B3	**B9**	**H9**	122.6
B1	**B9**	**H9**	121.8
B7	**B9**	**H9**	122.1
C8	**C9**	**C10**	115.9(4)
C8	**C9**	**C11**	116.8(4)
C10	**C9**	**C11**	127.2(4)
N2	**C10**	**C9**	121.1(4)
N2	**C10**	**C26**	114.0(3)
C9	**C10**	**C26**	124.9(4)
C26	**B10**	**C25**	58.0(2)
C26	**B10**	**B1**	106.1(3)
C25	**B10**	**B1**	105.9(3)
C26	**B10**	**B9**	106.0(3)
C25	**B10**	**B9**	58.9(2)
B1	**B10**	**B9**	60.5(3)
C26	**B10**	**B2**	58.6(3)
C25	**B10**	**B2**	105.2(3)
B1	**B10**	**B2**	60.6(3)
B9	**B10**	**B2**	108.6(4)
C26	**B10**	**H10**	123.7
C25	**B10**	**H10**	124.0
B1	**B10**	**H10**	122.1
B9	**B10**	**H10**	121.6
B2	**B10**	**H10**	122.0
C12	**C11**	**C16**	119.3(4)
C12	**C11**	**C9**	118.8(4)
C16	**C11**	**C9**	121.7(4)
C11	**C12**	**C13**	120.5(4)
C11	**C12**	**H12A**	119.8
C13	**C12**	**H12A**	119.8
C12	**C13**	**C14**	119.4(4)
C12	**C13**	**H13A**	120.3
C14	**C13**	**H13A**	120.3
C15	**C14**	**C13**	120.6(4)
C15	**C14**	**Br1**	120.4(4)
C13	**C14**	**Br1**	119.0(4)
C16	**C15**	**C14**	119.5(4)
C16	**C15**	**H15A**	120.2
C14	**C15**	**H15A**	120.2
C15	**C16**	**C11**	120.6(4)
C15	**C16**	**H16A**	119.7
C11	**C16**	**H16A**	119.7

C18	**C17**	**Pt1**	177.0(4)
C17	**C18**	**C19**	176.0(4)
C24	**C19**	**C20**	117.7(4)
C24	**C19**	**C18**	120.9(4)
C20	**C19**	**C18**	121.4(4)
C21	**C20**	**C19**	120.2(5)
C21	**C20**	**H20A**	119.9
C19	**C20**	**H20A**	119.9
C22	**C21**	**C20**	121.1(5)
C22	**C21**	**H21A**	119.4
C20	**C21**	**H21A**	119.4
C23	**C22**	**C21**	118.9(5)
C23	**C22**	**H22A**	120.5
C21	**C22**	**H22A**	120.5
C22	**C23**	**C24**	120.9(6)
C22	**C23**	**H23A**	119.6
C24	**C23**	**H23A**	119.6
C19	**C24**	**C23**	121.3(5)
C19	**C24**	**H24A**	119.4
C23	**C24**	**H24A**	119.4
C27	**C25**	**C26**	119.0(3)
C27	**C25**	**B7**	122.2(4)
C26	**C25**	**B7**	110.4(3)
C27	**C25**	**B9**	119.0(3)
C26	**C25**	**B9**	110.4(3)
B7	**C25**	**B9**	63.5(3)
C27	**C25**	**B10**	115.6(3)
C26	**C25**	**B10**	60.8(2)
B7	**C25**	**B10**	113.6(4)
B9	**C25**	**B10**	61.7(3)
C27	**C25**	**B6**	116.8(3)
C26	**C25**	**B6**	63.6(2)
B7	**C25**	**B6**	61.6(3)
B9	**C25**	**B6**	116.0(3)
B10	**C25**	**B6**	116.4(3)
C10	**C26**	**C25**	117.4(3)
C10	**C26**	**B8**	118.1(4)
C25	**C26**	**B8**	110.2(3)
C10	**C26**	**B2**	125.7(3)
C25	**C26**	**B2**	110.6(3)
B8	**C26**	**B2**	62.2(3)
C10	**C26**	**B10**	123.2(3)
C25	**C26**	**B10**	61.1(2)
B8	**C26**	**B10**	113.2(3)
B2	**C26**	**B10**	62.2(3)
C10	**C26**	**B6**	108.6(3)
C25	**C26**	**B6**	62.1(2)
B8	**C26**	**B6**	62.8(3)
B2	**C26**	**B6**	115.3(3)
B10	**C26**	**B6**	115.4(3)
C25	**C27**	**H27A**	109.5
C25	**C27**	**H27B**	109.5
H27A	**C27**	**H27B**	109.5
C25	**C27**	**H27C**	109.5
H27A	**C27**	**H27C**	109.5
H27B	**C27**	**H27C**	109.5