

## Supporting Information:

### Platinum(IV) centres with agostic interactions from either $sp^2$ or $sp^3$ C-H bonds.

Sarah H Crosby, Robert J Deeth, Guy J Clarkson and Jonathan P Rourke\*

Department of Chemistry, Warwick University, Coventry. UK CV4 7AL.

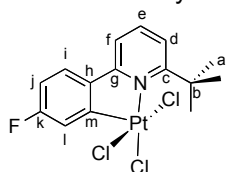
## Experimental

### General Considerations.

All chemicals were used as supplied, unless noted otherwise. All NMR spectra were obtained on a Bruker Avance, 400, 500 or 700 MHz spectrometer and  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts are referenced to external TMS, assignments being made with the use of decoupling, nOe and the HMBC, HMQC, DEPT and COSY pulse sequences.  $^{19}\text{F}$  chemical shifts are quoted from the directly observed signals and are referenced to external  $\text{CFCl}_3$ .  $^1\text{H}$ - $^{195}\text{Pt}$  correlation spectra were recorded using a variant of the HMBC pulse sequence with the  $^{195}\text{Pt}$  chemical shifts quoted taken from the 2D HETCOR spectra and referenced to external  $\text{Na}_2\text{PtCl}_6$ . All accurate mass spectra were run on a Bruker micrOTOF and Bruker MaXis mass spectrometer and X-ray crystal structures were collected on an Oxford Diffraction Gemini four-circle system with Ruby CCD area detector. Dichloro(phenyl)- $\lambda^3$ -iodane (often referred to as iodobenzene dichloride) was made via a literature route (R. T. Taylor, T. A. Stevenson, *Tetrahedron Lett.* **1988**, 29, 2033). Complexes 1 and 3 were synthesised as previously described (S H Crosby, G J Clarkson and J P Rourke. *J. Am. Chem. Soc.*, 2009, **131**, 14142)

### Synthesis of Complex 2.

To a  $\text{CDCl}_3$  solution of complex 1 (5 mg) in an NMR tube was added 1 eq dichloro(phenyl)- $\lambda^3$ -iodane and the reaction observed to go to completion within 10 minutes. The solvent was removed and the product washed with petroleum ether (40-60) to give a pure compound, 2 (5mg, 86%). Crystals of 2 suitable for single crystal analysis were formed by slow evaporation of solvent from a chloroform solution.



$\delta_{\text{H}}$  (700 MHz, 298 K,  $\text{CDCl}_3$ ): 7.93 (1H, t,  $^3J = 8$  Hz,  $\text{H}_e$ ), 7.71 (1H, d,  $^3J = 8$  Hz,  $\text{H}_f$ ), 7.48 (1H, d,  $^3J = 8$  Hz,  $\text{H}_d$ ), 7.40 (1H, dd,  $^3J = 8.6$  Hz,  $^4J_{\text{H-F}} = 5.5$  Hz,  $\text{H}_i$ ), 7.31 (1H, dd,  $^3J_{\text{H-F}} = 8.3$  Hz,  $^4J = 2.4$  Hz,  $^3J_{\text{H-Pt}} = 42$  Hz,  $\text{H}_l$ ), 7.00 (1H, td,  $^3J_{\text{H-H, H-F}} = 8.2$  Hz,  $^4J = 2.4$  Hz,  $\text{H}_j$ ), 1.84 (9H, s,  $J_{\text{H-Pt}} = 5$  Hz,  $\text{H}_a$ ) ppm.

$\delta_{\text{C}}$  (100 MHz, 298 K,  $\text{CDCl}_3$ ): 141.2 ( $\text{C}_e$ ), 126.4 (d,  $^3J_{\text{C-F}} = 10$  Hz,  $\text{C}_i$ ), 124.4 ( $\text{C}_{\text{d/f}}$ ), 119.5 ( $\text{C}_l$ ), 119.3 ( $^3J_{\text{C-Pt}} = 29$  Hz,  $\text{C}_{\text{b/d}}$ ), 115.6 (d,  $^2J_{\text{C-F}} = 23$  Hz,  $\text{C}_j$ ), 32.3 ( $J_{\text{C-Pt}} = 21$  Hz,  $\text{C}_a$ ) ppm.

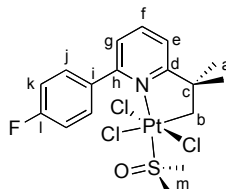
$\delta_{\text{F}}$  (375 MHz, 298 K,  $\text{CDCl}_3$ ): -98.8 ( $^4J_{\text{F-Pt}} = 33$  Hz) ppm.

$\delta_{\text{Pt}}$ : -1016 ppm.

Accurate Mass: 549.9770 calculated for  $\text{C}_{15}\text{H}_{15}^{35}\text{Cl}_3\text{FNNa}^{194}\text{Pt} = (\text{M}+\text{Na})^+$  549.9773

### Synthesis of Complexes 4 and 5.

Complex 3 (5 mg) was dissolved in  $\text{CDCl}_3$  in an NMR tube and 1 eq of dichloro(phenyl)- $\lambda^3$ -iodane added at  $-40^\circ\text{C}$ . The reaction was followed by both  $^1\text{H}$ - and  $^{19}\text{F}$ -NMR and the reaction proceeded to give a single product, 4.



Spectroscopic data for 4

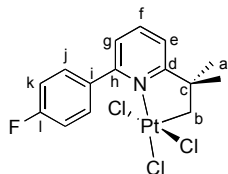
$\delta_{\text{H}}$  (500 MHz, 233 K,  $\text{CDCl}_3$ ): 7.88 (1H, t,  $^3J = 7.8$  Hz,  $\text{H}_f$ ), 7.55 (2H, dd,  $^3J = 8.6$  Hz,  $^4J_{\text{H-F}} = 5.2$  Hz,  $\text{H}_j$ ), 7.30 (1H, dd,  $^3J = 7.5$  Hz,  $^4J = 1.0$  Hz,  $\text{H}_g$ ), 7.21 (1H, dd,  $^3J = 7.6$  Hz,  $^4J = 1.4$  Hz,  $\text{H}_e$ ), 7.11 (2H, t,  $^3J_{\text{H-H, H-F}} = 8.7$  Hz,  $\text{H}_k$ ), 4.11 (2H, s,  $^2J_{\text{H-Pt}} = 72.5$  Hz,  $\text{H}_b$ ), 3.58 (6H, s,  $^3J_{\text{H-Pt}} = 15.5$  Hz,  $\text{H}_m$ ), 1.56 (6H, s,  $\text{H}_a$ ) ppm.

$\delta_{\text{C}}$  (100 MHz, 233 K,  $\text{CDCl}_3$ ): 140.9 ( $\text{C}_f$ ), 131.9 ( $\text{C}_j$ ), 122.6 ( $\text{C}_g$ ), 128.7 ( $\text{C}_e$ ), 115.0 ( $\text{C}_k$ ), 53.7 ( $\text{C}_b$ ), 40.7 ( $\text{C}_m$ ), 33.0 ( $\text{C}_a$ ) ppm. (Aromatic protons taken from HMQC)

$\delta_F$  (375 MHz, 253 K,  $CDCl_3$ ): -111.4 ppm.

$\delta_{Pt}$ : -1568 ppm.

On warming to room temperature this product, 4, was observed *via*  $^1H$ -NMR to transform into a new product, 5. The solvent was removed and the product washed with petroleum ether (40-60) to give a pure complex, 5 (4mg).



Spectroscopic data for 5

$\delta_H$  (500 MHz, 298 K,  $CDCl_3$ ): 8.04 (2H, dd,  $^3J = 8.8$  Hz,  $^4J_{H-F} = 5$  Hz,  $H_i$ ), 8.03 (1H, t,  $^3J = 7.8$  Hz,  $H_f$ ), 7.52 (1H, dd,  $^3J = 7.8$  Hz,  $^4J = 1.3$  Hz,  $H_g$ ), 7.36 (1H, dd,  $^3J = 8$  Hz,  $^4J = 1.5$  Hz,  $H_e$ ), 7.35 (2H, t,  $^3J_{H-H, H-F} = 8.5$  Hz,  $H_k$ ), 5.25 (2H, s,  $^2J_{H-Pt} = 87$  Hz,  $H_b$ ), 1.63 (6H, s,  $H_a$ ) ppm.

$\delta_C$  (100 MHz, 298 K,  $CDCl_3$ ): 172.3 ( $C_d$ ), 164.4 (d,  $^1J_{C-F} = 254$  Hz,  $C_i$ ), 158.2 ( $C_h$ ), 141.1 ( $C_f$ ), 131.7 (d,  $^4J_{C-F} = 4$  Hz,  $C_j$ ), 130.8 (d,  $^3J_{C-F} = 8.5$ ,  $J_{C-Pt} = 7$  Hz,  $C_j$ ), 126.1 ( $^3J_{C-Pt} = 24.5$  Hz,  $C_g$ ), 122.6 ( $^3J_{C-Pt} = 37.5$  Hz,  $C_e$ ), 118.0 (d,  $^2J_{C-F} = 20$  Hz,  $C_k$ ), 55.6 ( $^1J_{C-Pt} = 487$  Hz,  $C_b$ ), 51.9 ( $C_c$ ), 29.7 ( $^3J_{C-Pt} = 17.5$  Hz,  $C_a$ ) ppm.

$\delta_F$  (375 MHz, 298 K,  $CDCl_3$ ): -107.1 ppm.

$\delta_{Pt}$ : -851 ppm.

Accurate Mass: 549.9774 calculated for  $C_{15}H_{15}^{35}Cl_3FNNa^{194}Pt = (M+Na)^+$  549.9773, 492.0189 calculated for  $C_{15}H_{15}^{35}Cl_2FN^{194}Pt = (M-Cl)^+$  492.0187

### Comparison of coupling constants

The values (Hz) of  $^1J(Pt-C_b)$  and  $^2J(Pt-H_b)$  for complexes 3, 4 and 5 are as follows:

Complex	$^1J(Pt-C_b)$	$^2J(Pt-H_b)$
3	702	59
4	-	72
5	487	87

The  $^1J(Pt-C_b)$  follows the expected trend of decreasing with increasing oxidation state. However, the  $^2J(Pt-H_b)$  does not. We suggest that this apparently counter-intuitive change is down to the angular dependence of the  $^2J(Pt-H_b)$ , whereby a change in geometry alters the Pt-C-H bond angle, affecting the coupling.

## Crystallographic data for sc14 (Complex 2)

The asymmetric unit contains the trichloro Pt complex. There are 4 in the unit cell. The hydrogens on C16 were located in a difference map and their position allowed to refine freely but given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl hydrogen atoms) times the equivalent isotropic displacement parameter of C16 to which they are attached.

Bond lengths and angles for the C16 methyl are

1.0409 (0.0337) Angstroms C16 - H16A

1.0342 (0.0327) Angstroms C16 - H16B

0.9290 (0.0345) Angstroms C16 - H16C

112.22 ( 1.82)  $C_{13} - C_{16} - H_{16A}$

103.64 ( 1.75)  $C_{13} - C_{16} - H_{16B}$

107.45 ( 2.12)  $C_{13} - C_{16} - H_{16C}$

(An idealized methyl group would be 0.98 Angstroms and about 108 degrees)

Pt1 distances to C16 and H16A are shown below

2.1568 (0.0316) H16A - Pt1

2.7212 (0.0029) C16 - Pt1

Torsion angles

17.55 ( 0.37) degrees N1 - C2 - C13 - C16

Short contacts

Specified hydrogen bonds (with esds except fixed and riding H)

D-H	H...A	D...A	<(DHA)	
0.95	2.78	3.707(3)	167.0	C3-H3A...C12_\$1
0.95	2.47	3.344(3)	152.3	C9-H9A...F10_\$2

There is no meaningful pi stacking as the molecules cant seem to get close enough because the three chlorines are fending them off.

#### Crystal Data

C<sub>15</sub>H<sub>15</sub>Cl<sub>3</sub>F<sub>3</sub>NPt, M = 529.72, Monoclinic, space group P2(1)/c  
a = 13.0861(2), b = 8.07835(10), c = 15.9059(3) Å,  
alpha = 90 deg., beta = 111.7518(19) deg., gamma = 90 deg.,  
U = 1561.75(4) Å<sup>3</sup> (by least squares refinement on 11638 reflection positions),  
T = 100(2)K, lambda = 0.71073 Å, Z = 4,  
D(cal) = 2.253 Mg/m<sup>3</sup>, F(000) = 1000.  
mu(MoK-alpha) = 9.499 mm<sup>-1</sup>.  
Crystal character: colourless plate.  
Crystal dimensions 0.15 x 0.15 x 0.01 mm,

#### Data Collection and Processing.

Oxford Diffraction Gemini four-circle system with Ruby CCD area detector.  
The crystal was held at 100(2)K with the Oxford Cryosystem Cobra.  
Maximum theta was 30.82 deg.  
The hkl ranges were -14/ 18, -11/ 11, -22/ 20.  
18193 reflections measured, 4551 unique [R(int) = 0.0402].  
Absorption correction by Semi-empirical from equivalents;  
minimum and maximum transmission factors: 0.42; 1.00.  
no crystal decay

#### Structure Analysis and Refinement.

Systematic absences indicated space group P2(1)/c and shown to be correct by successful refinement.

The structure was solved by direct methods using SHELXS (Sheldrick, 1990) (TREF) with additional light atoms found by Fourier methods.

Hydrogen atoms were added at calculated positions and refined using a riding model with freely rotating methyl groups except the hydrogens on C16 which were located in a difference map and their position allowed to refine freely. Anisotropic displacement parameters were used for all non-H atoms; H-atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl hydrogen atoms) times the equivalent isotropic displacement parameter of the atom to which the H-atom is attached.

The absolute structure of the individual crystal chosen was checked by refinement of a delta-f" multiplier.

Floating origin constraints were generated automatically.

The weighting scheme was calc  $w=1/[\sigma^2(F_o^2)+(0.0207P)^2+0.0000P]$  where  $P=(F_o^2+2F_c^2)/3$ .

Goodness-of-fit on F<sup>2</sup> was 0.972,

R1[for 3917 reflections with I > 2sigma(I)] = 0.0204, wR2 = 0.0428.

Data / restraints / parameters 4551/ 0/ 201.

Largest difference Fourier peak and hole 1.400 and -1.780 e.Å<sup>-3</sup> .

Refinement used SHELXL 97 (Sheldrick, 1997).

The Oxford Diffraction Gemini XRD system was obtained through the Science City Advanced Materials project: Creating and Characterising Next Generation Advanced Materials, with support from Advantage West Midlands (AWM) and part funded by the European Regional Development Fund (ERDF)

#### References

For relevant information for the SHELXTL suite of programmes used to solve, refine and produce the files for this structure, please refer to "A Short History of Shelx, G. M. Sheldrick, Acta Cryst. 2008, A64, 112-122"

Use Mercury (Free from CCDC at [www.ccdc.cam.ac.uk/products/mercury](http://www.ccdc.cam.ac.uk/products/mercury)) to view the structure.

Table 1. Atomic coordinates ( x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for sc14. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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x	y	z	U(eq)
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Pt(1)	2291.6(1)	5633.8(1)	4156.1(1)	10(1)
N(1)	2177.6(18)	7518(3)	3281.7(14)	10(1)
Cl(1)	2400.1(6)	3488.7(8)	5134.8(4)	17(1)
Cl(2)	739.3(5)	6614.1(8)	4364.9(4)	14(1)
C(2)	1641(2)	7436(3)	2367.0(17)	12(1)
Cl(3)	3808.7(6)	4663.3(8)	3905.9(5)	17(1)
C(3)	1653(2)	8813(3)	1856.5(18)	15(1)
C(4)	2172(2)	10263(3)	2267.6(19)	16(1)
C(5)	2691(2)	10325(3)	3196.2(19)	15(1)
C(6)	2699(2)	8927(3)	3698.1(18)	13(1)
C(7)	3275(2)	8766(3)	4678.9(18)	13(1)
C(8)	3894(2)	10035(4)	5240.1(19)	15(1)
C(9)	4450(2)	9764(4)	6155.9(19)	17(1)
F(10)	4960.3(14)	7931(2)	7388.0(10)	26(1)
C(10)	4398(2)	8207(4)	6490.4(18)	18(1)
C(11)	3797(2)	6911(4)	5980.2(18)	15(1)
C(12)	3237(2)	7234(3)	5070.4(18)	13(1)
C(13)	1080(2)	5831(3)	1899.5(17)	12(1)
C(14)	-62(2)	6261(4)	1182.0(19)	17(1)
C(15)	1804(2)	5044(4)	1430.7(19)	15(1)
C(16)	864(3)	4547(4)	2524.2(19)	16(1)

Table 2. Bond lengths [Å] and angles [deg] for sc14.

Pt(1)-C(12)	1.996(3)
Pt(1)-N(1)	2.029(2)
Pt(1)-Cl(1)	2.2984(6)
Pt(1)-Cl(3)	2.3021(7)
Pt(1)-Cl(2)	2.3161(6)
Pt(1)-H(16A)	2.16(3)
N(1)-C(2)	1.363(3)
N(1)-C(6)	1.366(3)
C(2)-C(3)	1.381(4)
C(2)-C(13)	1.539(4)
C(3)-C(4)	1.389(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.379(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.380(4)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.465(4)
C(7)-C(12)	1.394(4)
C(7)-C(8)	1.403(4)
C(8)-C(9)	1.383(4)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.377(4)
C(9)-H(9A)	0.9500
F(10)-C(10)	1.361(3)
C(10)-C(11)	1.379(4)
C(11)-C(12)	1.383(4)
C(11)-H(11A)	0.9500
C(13)-C(16)	1.533(4)
C(13)-C(15)	1.544(4)
C(13)-C(14)	1.546(4)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	1.04(3)

C(16)-H(16B)	1.03(3)
C(16)-H(16C)	0.93(3)
C(12)-Pt(1)-N(1)	83.21(10)
C(12)-Pt(1)-Cl(1)	97.41(8)
N(1)-Pt(1)-Cl(1)	179.30(7)
C(12)-Pt(1)-Cl(3)	90.30(8)
N(1)-Pt(1)-Cl(3)	89.20(6)
Cl(1)-Pt(1)-Cl(3)	91.12(2)
C(12)-Pt(1)-Cl(2)	90.78(8)
N(1)-Pt(1)-Cl(2)	89.79(6)
Cl(1)-Pt(1)-Cl(2)	89.88(2)
Cl(3)-Pt(1)-Cl(2)	178.42(2)
C(12)-Pt(1)-H(16A)	164.0(9)
N(1)-Pt(1)-H(16A)	87.3(8)
Cl(1)-Pt(1)-H(16A)	92.2(8)
Cl(3)-Pt(1)-H(16A)	76.7(9)
Cl(2)-Pt(1)-H(16A)	102.1(9)
C(2)-N(1)-C(6)	121.7(2)
C(2)-N(1)-Pt(1)	124.98(17)
C(6)-N(1)-Pt(1)	113.34(17)
N(1)-C(2)-C(3)	118.4(2)
N(1)-C(2)-C(13)	121.4(2)
C(3)-C(2)-C(13)	120.1(2)
C(2)-C(3)-C(4)	120.8(2)
C(2)-C(3)-H(3A)	119.6
C(4)-C(3)-H(3A)	119.6
C(5)-C(4)-C(3)	119.7(3)
C(5)-C(4)-H(4A)	120.2
C(3)-C(4)-H(4A)	120.2
C(4)-C(5)-C(6)	119.0(3)
C(4)-C(5)-H(5A)	120.5
C(6)-C(5)-H(5A)	120.5
N(1)-C(6)-C(5)	120.4(2)
N(1)-C(6)-C(7)	114.2(2)
C(5)-C(6)-C(7)	125.4(3)
C(12)-C(7)-C(8)	118.2(2)
C(12)-C(7)-C(6)	117.7(2)
C(8)-C(7)-C(6)	124.1(3)
C(9)-C(8)-C(7)	120.6(3)
C(9)-C(8)-H(8A)	119.7
C(7)-C(8)-H(8A)	119.7
C(10)-C(9)-C(8)	118.0(3)
C(10)-C(9)-H(9A)	121.0
C(8)-C(9)-H(9A)	121.0
F(10)-C(10)-C(9)	118.1(2)
F(10)-C(10)-C(11)	117.5(3)
C(9)-C(10)-C(11)	124.4(3)
C(10)-C(11)-C(12)	115.9(3)
C(10)-C(11)-H(11A)	122.0
C(12)-C(11)-H(11A)	122.0
C(11)-C(12)-C(7)	122.8(3)
C(11)-C(12)-Pt(1)	125.8(2)
C(7)-C(12)-Pt(1)	111.38(19)
C(16)-C(13)-C(2)	115.2(2)
C(16)-C(13)-C(15)	109.1(2)
C(2)-C(13)-C(15)	108.1(2)
C(16)-C(13)-C(14)	105.7(2)
C(2)-C(13)-C(14)	109.0(2)
C(15)-C(13)-C(14)	109.5(2)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	112.2(18)
C(13)-C(16)-H(16B)	103.6(17)
H(16A)-C(16)-H(16B)	105(2)
C(13)-C(16)-H(16C)	107(2)
H(16A)-C(16)-H(16C)	118(3)
H(16B)-C(16)-H(16C)	110(3)

Table 3. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for sc14.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
Pt(1)	11(1)	10(1)	9(1)	0(1)	4(1)	1(1)
N(1)	10(1)	10(1)	11(1)	1(1)	6(1)	1(1)
Cl(1)	22(1)	14(1)	15(1)	4(1)	6(1)	1(1)
Cl(2)	14(1)	20(1)	11(1)	1(1)	6(1)	3(1)
C(2)	9(1)	15(1)	12(1)	-2(1)	5(1)	1(1)
Cl(3)	14(1)	19(1)	19(1)	-3(1)	7(1)	3(1)
C(3)	17(1)	20(1)	9(1)	1(1)	4(1)	2(1)
C(4)	20(2)	13(1)	16(1)	3(1)	9(1)	2(1)
C(5)	17(1)	13(1)	16(1)	1(1)	8(1)	1(1)
C(6)	13(1)	12(1)	16(1)	-1(1)	9(1)	1(1)
C(7)	11(1)	15(1)	13(1)	-2(1)	5(1)	1(1)
C(8)	15(1)	15(1)	18(1)	-3(1)	10(1)	-2(1)
C(9)	15(1)	20(1)	14(1)	-8(1)	3(1)	-2(1)
F(10)	30(1)	30(1)	11(1)	-1(1)	-1(1)	-1(1)
C(10)	16(1)	25(2)	11(1)	-2(1)	3(1)	5(1)
C(11)	16(1)	18(1)	14(1)	1(1)	7(1)	5(1)
C(12)	10(1)	13(1)	14(1)	-3(1)	5(1)	2(1)
C(13)	12(1)	14(1)	11(1)	-3(1)	6(1)	-3(1)
C(14)	14(1)	20(1)	16(1)	-3(1)	4(1)	-1(1)
C(15)	18(2)	14(1)	17(1)	-1(1)	11(1)	0(1)
C(16)	20(2)	16(1)	12(1)	-1(1)	7(1)	-4(1)

Table 4. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for sc14.

	x	y	z	U(eq)
H(3A)	1302	8769	1216	18
H(4A)	2169	11207	1911	19
H(5A)	3037	11314	3486	18
H(8A)	3932	11090	4989	18
H(9A)	4856	10625	6542	21
H(11A)	3770	5859	6238	18

H(14A)	28	7020	734	25
H(14B)	-514	6789	1478	25
H(14C)	-424	5245	879	25
H(15A)	1926	5848	1016	23
H(15B)	1433	4065	1089	23
H(15C)	2513	4718	1889	23
H(16A)	1590(30)	4060(40)	2990(20)	24
H(16B)	490(30)	3580(40)	2090(20)	24
H(16C)	370(30)	5010(40)	2750(20)	24

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## Computation studies on 5

Studies were conducted using both B3LYP/LANL2DZ and MP2/LANL2DZ levels of theory, using Gaussian 03.

Gaussian 03: Gaussian 03, Revision D.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

XYZ coordinates for lowest energy conformer  
MP2/LANL2DZ: E = -894.690238 a.u.

#	Symbol	X	Y	Z
1	Pt	0.191420	-0.814383	0.031414
2	N	0.738181	1.140317	-0.175679
3	C	-0.228576	2.110083	-0.378869
4	C	0.171728	3.463223	-0.519882
5	C	2.077257	1.421656	-0.031397
6	C	2.506846	2.771606	-0.176959
7	C	1.554001	3.793623	-0.430231
8	C	-1.639271	1.616909	-0.368505
9	C	3.002445	0.244251	0.317709
10	C	3.773360	0.582181	1.645265
11	C	2.169785	-1.073711	0.573449
12	C	4.022642	0.014833	-0.852384
13	C	-2.593983	2.226918	0.500725
14	C	-3.900318	1.681412	0.622413
15	C	-4.216767	0.525488	-0.131164
16	C	-3.312770	-0.092686	-1.021773

17	C	-2.008321	0.469023	-1.149363
18	F	-5.521778	-0.027858	0.008179
19	Cl	-0.437345	-0.273062	2.300310
20	Cl	-0.460367	-3.094483	0.300745
21	Cl	0.838671	-1.202553	-2.280276
22	H	4.705907	-0.812489	-0.586144
23	H	4.633128	0.921577	-1.026194
24	H	3.489501	-0.247488	-1.781317
25	H	4.408848	-0.276866	1.928100
26	H	3.058550	0.778000	2.465335
27	H	4.428934	1.464416	1.518801
28	H	-3.611382	-0.970301	-1.598967
29	H	1.878816	4.829893	-0.551448
30	H	3.568244	3.010392	-0.080590
31	H	-4.642757	2.112333	1.298069
32	H	-1.348157	0.092528	-1.936487
33	H	-2.301251	3.077063	1.123615
34	H	-0.585715	4.226972	-0.711125
35	H	2.127979	-1.338886	1.642572
36	H	2.522673	-1.913978	-0.045821

XYZ coordinates and energy for the structure corresponding to barrier  
MP2/LANL2DZ: E = -894.687936

#	Symbol	X	Y	Z
1	Pt	-0.205414	-0.823692	0.010628
2	N	-0.746172	1.134458	-0.028791
3	C	0.244384	2.095348	-0.076495
4	C	-0.126367	3.462064	-0.109963
5	C	-2.089687	1.418200	-0.007989
6	C	-2.492266	2.783947	-0.042748
7	C	-1.510274	3.808034	-0.095158
8	C	1.652053	1.568897	-0.062261
9	C	-3.047092	0.218851	0.053047
10	C	-3.953123	0.221307	-1.228996
11	C	-2.248214	-1.141920	0.108587
12	C	-3.925900	0.330487	1.349448
13	C	2.287896	1.190176	-1.287811
14	C	3.624400	0.703163	-1.275214
15	C	4.287130	0.614658	-0.030304
16	C	3.692979	0.979400	1.200095
17	C	2.357504	1.464346	1.178872
18	F	5.628442	0.130239	-0.012616
19	Cl	-0.332789	-0.821460	-2.406579



20	Cl	0.480165	-3.105349	0.058293
21	Cl	-0.111146	-0.648155	2.421387
22	H	-4.615074	-0.532013	1.403337
23	H	-4.534278	1.254605	1.343767
24	H	-3.282024	0.327022	2.247364
25	H	-4.652037	-0.634102	-1.188221
26	H	-3.329539	0.128314	-2.135820
27	H	-4.551459	1.149795	-1.293938
28	H	4.250884	0.869829	2.132457
29	H	-1.813388	4.857626	-0.122728
30	H	-3.556131	3.031441	-0.027871
31	H	4.130492	0.390662	-2.191040
32	H	1.859326	1.733639	2.112456
33	H	1.744650	1.265644	-2.231412
34	H	0.655465	4.223767	-0.148238
35	H	-2.461820	-1.786692	-0.758720
36	H	-2.392017	-1.672287	1.063368