Supplementary Material (ESI) for Chemical Communications

SUPPORTING INFORMATION

for

Unusual Reactivities of N-Heterocyclic Carbenes upon Coordination to the Platinum(II)-Dimethyl Moiety

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General Considerations. Unless stated otherwise all reactions were preformed in an MBraun drybox or under Schlenk techniques. Solvents were obtained from Sigma Aldrich and were dried and degassed as necessary utilizing conventional methods. (COD)$PtMe_2$ was obtained from Strem Chemicals and used as received. ^{Me}IMe,[1] ^{Me}IPr,[1] ICy,[2] IMes,[2] IPr[3] and I^{t}Bu[4] were synthesized by literature methods. ^{1}H and ^{13}C NMR were obtained on either a Burker 400 MHz or a Bruker 300 MHz NMR spectrometer. Spectra were referenced to benzene at δ 7.16 (^{13}C, δ 128.0), toluene at δ 2.04, or THF-d_8 at δ 3.58 (^{13}C, δ 67.6) ppm. Elemental Analyses were performed at the Universität Zürich, Organisch-chemisches Institut.

Synthesis of *cis*-Pt(^{Me}IMe)$_2$Me$_2$ (1). Toluene (3 mL) was added to the solids (COD)$PtMe_2$ (100 mg, 0.3 mmol) and ^{Me}IMe (75.2 mg, 0.6 mmol) in a reaction vial. The resulting solution was stirred for 20 minutes, and then the volatiles were removed in vacuo, yielding a white solid. The compound was washed with pentane (3 x 2 mL), affording 131 mg (92 %) of the desired complex. X-ray quality crystals were obtained by slow evaporation of a saturated CH_2Cl_2/pentane solution at room temperature. Anal. Calcd for $C_{16}H_{30}N_4Pt$ (MW 473.53): C, 40.58; H, 6.39; N, 11.83. Found: C, 40.72; H, 6.16; N, 11.89. ^{1}H NMR (C_6D_6, 400 MHz, δ): 3.53 (s, 12H, N(1,3)-C**H**$_3$), 1.45 (s, 12H, C(4,5)-C**H**$_3$), 1.08 (s, 6H, $^2J_{Pt}$ = 65.1 Hz, C**H**$_3$). ^{13}C NMR (C_6D_6, 400 MHz, δ): 187.3 (s, N-**C**-N), 122.6 (s, **C**(4,5)), 34.1 (s, $^3J_{Pt}$ = 47.2 Hz, N(1,3)-**C**H$_3$), 9.06 (s, C(4,5)-**C**H$_3$), -7.76 (s, $^1J_{Pt}$ = 553.9 Hz, **C**H$_3$).

Synthesis of *cis*-Pt(ICy)$_2$Me$_2$ (2). Benzene (25mL) was added to the solids (COD)$PtMe_2$ (200 mg, 0.6 mmol) and ICy (365 mg, 1.2 mmol) in a reaction vial. The resulting solution was stirred for 1 hour, and then the volatiles were removed in vacuo, yielding a white solid. The compound was washed with pentane (3 x 5 mL), affording 414 mg (85 %) of the desired complex. X-ray quality crystals were obtained by slow evaporation of a saturated CH_2Cl_2/pentane solution at room temperature. Anal. Calcd for $C_{32}H_{54}N_4Pt$ (MW 689.90): C, 55.71; H, 7.89; N, 8.12. Found: C, 56.28 ; H, 7.67 ; N, 8.13. ^{1}H NMR (C_6D_6, 400 MHz, δ): 6.50 (s, 4H, $^4J_{Pt}$ = 6.7 Hz. NC**H**=C**H**N), 5.37 (m, 4H, ICy-C**H**), 2.15

(m, 4H, *p*-ICy-C**H**$_2$), 1.82 (m, 4H, *p*-ICy-C**H**$_2$), (1.63 – 0.94 (m, 36H, *m*/*o*-ICy-C**H**$_2$), 0.89 (s, 6H, $^2J_{Pt}$ = 65.9 Hz, C**H**$_3$). ^{13}C NMR (CD_2Cl_2, 400 MHz, δ): 185.55 (s, $^1J_{CPt}$ = 1700.56Hz, N-C-N), 116.29 (s, $^3J_{CPt}$ = 44.0 Hz, NHC=CHN), 52.58 (s, SIPr-NCH_2CH_2N), 28.67 (s, SIPr-CH), 25.42 (s, SIPr-CH_3) 24.81 (s, SIPr-CH_3), -8.36 (s, $^1J_{CPt}$ = 1104.4 Hz, CH_3).

Synthesis of *cis*-Pt(^{Me}IPr)$_2$Me$_2$ (3). Toluene (10 mL) was added to the solids (COD)$PtMe_2$ (100 mg, 0.30 mmol) and ^{Me}IPr (108.2 mg, 0.60 mmol) in a reaction vial. The resulting solution was stirred for 1 h, and then the volatiles were removed in vacuo, yielding a light cream colored solid. The compound was washed with pentane (3 x 5 mL), affording 185.4 mg (89 %) of the desired complex. X-ray quality crystals were obtained by slow evaporation of a saturated CH_2Cl_2/pentane solution at room temperature. Anal. Calcd for $C_{24}H_{46}N_4Pt$ (MW 585.34): C, 49.21; H, 7.92; N, 9.57. Found: C, 49.49; H, 7.88; N, 9.67. ^{1}H NMR (tol-d^8, 400 MHz, δ): 6.36 (s, 4H, sept, *J* = 7.21 Hz, C**H**$(CH_3)_2$), 1.78 (s, 12H, s, C(4,5)-C**H**$_3$), 1.38 (d, 12H, *J* = 7.13 Hz, CH(C**H**$_3)_2$), 1.02 (d, 12H, *J* = 7.26 Hz, CH(C**H**$_3)_2$), 1.00 (s, 6H, $^2J_{Pt}$ = 65.6 Hz, Pt-C**H**$_3$). ^{13}C NMR (tol-d_8, 400 MHz, δ): 188.2 (s, N-**C**-N), 122.8 (s, $^3J_{Pt}$ = 17.5 Hz **C**(4,5)), 51.3 (s, $^3J_{Pt}$ = 52.8 Hz, **C**H$(CH_3)_2$), 22.6 (s, CH(**C**H$_3)_2$), 20.4 (s, CH(**C**H$_3)_2$) 10.2 (s, C(4,5)-**C**H$_3$), -7.75 (s, Pt-**C**H$_3$).

Synthesis of *cis*-Pt(IMes)$_2$Me$_2$ (4).[5] Benzene (25mL) was added to the solids (COD)$PtMe_2$ (200 mg, 0.6 mmol) and IMes (365 mg, 1.2 mmol) in a Schenk flask. The resulting colourless solution was stirred for 10 minutes, and then the volatiles were removed in vacuo, yielding a white solid. The compound was washed with pentane (3 x 5 mL), affording 380 mg (76 %) of the desired complex. X-ray quality crystals were obtained by slow evaporation of a saturated benzene/Et_2O solution at room temperature. Anal. Calcd for $C_{44}H_{54}N_4Pt$ (MW 833): C, 63.37; H, 6.53; N, 6.72. Found: C, 63.75 ; H, 6.72 ; N, 6.67 . ^{1}H NMR (C_6D_6, 400 MHz, δ): 6.68 (s, 4H, IMes-C**H**-Ar), 6.52 (s, 4H, IMes-C**H**-Ar), 6.13 (s, 4H, NC**H**=C**H**N), 2.38 (s, 12H, IMes-C**H**$_3$), 2.22 (s, 12H, IMes-C**H**$_3$), 1.87 (s, IMes-C**H**$_3$), 0.39 (s, 6H, $^2J_{Pt}$ = 68.1 Hz , Me). ^{13}C NMR (C_6D_6, 400 MHz, δ): 193.1 (s,N-C-N), 139.2 (s, SIPr-**C**), 136.8 (s, SIPr-**C**), 136.3 (s, SIPr-**C**), 135.8 (s,

SIPr-**C**), 130.23 (s, SIPr-**C**) 129.3 (s, overlapping with C_6D_6, SIPr-**C**), 123.3 (s, SIPr-N**C**H_2**C**H_2N), 21.6 (s, SIPr-**C**H), 20.4 (s, SIPr-**C**H_3), -0.03 (s, Pt-**C**H_3).

Synthesis of Pt(IMes)(IMes')Me (5).[5] Toluene (10 mL) was added to the solids (COD)$PtMe_2$ (50.0 mg, 0.15 mmol) and IMes (91.4 mg, 0.30 mmol) in a Schlenk flask. The sealed flask was removed from the glove box and attached to a Schlenk line under argon. The clear colorless solution was heated with stirring for 16 hr at 60 ^oC. The final color of the solution was light yellow. The solvent was removed in vacuo and washed with cold pentane (3 x 2 mL) followed by one wash with cold toluene (1 mL) to yield 46.2 mg (46 %) of an off white colored powder. X-ray quality crystals were obtained by slow evaporation of a saturated benzene/Et_2O solution at room temperature. Anal. Calcd for $C_{43}H_{50}N_4Pt$ (MW 817.96) C, 63.14; H, 6.16; N, 6.85. Found: C, 63.57; H, 6.34; N, 6.34. ^{1}H NMR (C_6D_6, 400 MHz, δ): 7.00 (s, Mes-CH); 6.76 (s, 1H, Mes-CH); 6.70 (s, 1H, Mes-CH); 6.64 (s, 1H, Mes-CH); 6.60 (s, 1H, Mes-CH); 6.57 (s, 2H, CH=CH) 6.55 (s, 1H, Mes-CH); 6.47 (s, 1H, Mes-CH); 6.15 (s, 1H, Mes-CH); 6.09 (d, 1H); 6.00 (d, 1H, J = 2.2 Hz); 2.59 (s, 3H, Mes-CH_3); 2.40 (s, 3H, Mes-CH_3); 2.25 (s, 3H, Mes-CH_3); 2.23 (s, 6H, Mes-CH_3); 2.22 (s, 2H, Pt-CH_2); 2.15 (s, 3H, Mes-CH_3); 1.97 (s, 3H, Mes-CH_3); 1.92 (s, 3H, Mes-CH_3); 1.83 (s, 3H, Mes-CH_3); 1.39 (s, 3H, Mes-CH_3); 0.66 (s, 3H, $^2J_{Pt}$ =70.0 Hz, Pt-Me). ^{13}C NMR (C_6D_6, 400 MHz, δ): 193.7 (s, $^1J_{Pt}$ = 887.7 Hz, N-C-N), 188.1 (s, $^1J_{Pt}$ = 945.08 Hz, N-C-N) 138.89 (s, Mes-**C**), 138.72 (s, Mes-**C**), 138.33(s, Mes-**C**), 138.13 (s, Mes-**C**), 137.72 (s, Mes-**C**), 136.95 (s, Mes-**C**), 136.58 (s, Mes-**C**), 136.42 (s, Mes-**C**), 136.26 (s, Mes-**C**), 135.60 (s, Mes-**C**), 134.05 (s, Mes-**C**), 133.98 (s, Mes-**C**), 130.85 (s, Mes-**C**), 130.05 (s, Mes-**C**), 129.09 (s, Mes-**C**), 128.90 (s, Mes-**C**), 126.95 (s, Mes-**C**), 123.35 (s, NCH=CHN), 122.30 (s, NCH=CHN), 120.99 (s, NCH=CHN) 120.43 (s, NCH=CHN), 23.04 (s, Pt-CH_2-Mes), 21.86 (s, Mes-**C**H_3), 21.80 (s, Mes-**C**H_3), 21.51 (s, Mes-**C**H_3), 21.26 (s, Mes-**C**H_3), 20.09 (s, Mes-**C**H_3), 19.83 (s, Mes-**C**H_3), 19.56 (s, Mes-**C**H_3), 19.27 (s, Mes-**C**H_3), 19.08 (s, Mes-**C**H_3), 18.82 (s, Mes-**C**H_3), -4.85 (s, Pt-Me) .

Synthesis of Pt(IPr)$_2$ (6). Toluene (25mL) was added to the solids (COD)$PtMe_2$ (200 mg, 0.6 mmol) and IPr (466 mg, 1.2 mmol) in a Schlenk flask. The resulting yellow

solution was heated at 80 ^{o}C for 12 h, and then the volatiles were removed in vacuo, yielding a bright yellow solid. The compound was washed with pentane (3 x 5 mL), affording 390 mg (67 %) of the desired complex. X-ray quality crystals were obtained by slow evaporation of a saturated Et_2O solution at room temperature. Anal. Calcd for $C_{54}H_{72}N_4Pt$ (MW 972.28): C, 66.71; H, 7.96; N, 5.76. Found: C, 66.65; H, 8.09; N, 5.92. ^{1}H NMR (C_6D_6, 400 MHz, δ): 7.31 (m, 4H, *p*-Ar-**H**), 7.09 (d, 8H, *J* = 7.6 Hz, *o*-Ar-**H**) 6.23 (s, 4H, C(4,5)-**H**), 2.94 (sept, 4H, *J* = 6.9 Hz, C**H**$(CH_3)_2$), 1.24 (d, 24H, *J* = 6.9 Hz, CH(C**H**$_3)_2$), 1.12 (d, 24H, *J* = 7.0 Hz, CH(C**H**$_3)_2$). ^{13}C NMR (C_6D_6, 400 MHz, δ): 198.3 (s, $^1J_{CPt}$ = 1880 Hz, N-C-N), 146.27 (s, IPr-**C**), 139.43 (s, IPr-**C**), 129.03 (s, overlapping with C_6D_6, IPr-**C**), 123.79 (s, IPr-**C**), 121.59 (s, N**C**H=**C**HN), 29.10 (s, IPr-**C**H), 25.47 (s, IPr-**C**H_3), 24.41 (s, IPr-**C**H_3).

Synthesis of Pt(*n*I^{t}Bu)(*a*I^{t}Bu)$_2$Me$_2$ (7). Et_2O (10 mL) was added to the solids (COD)$PtMe_2$ (200 mg, 0.6 mmol) and I^{t}Bu (21.6 mg, 1.2 mmol) in a reaction vial. The resulting solution was stirred for 2 weeks or until an appearance of a white solid. The solution was decanted and the white precipitate was washed with Et_2O (3 x 5 mL), affording 157 mg (51 % yield) of Pt(*n*I^{t}Bu)(*a*I^{t}Bu)$_2$Me$_2$. X-ray quality crystals were obtained by slow evaporation of a saturated CH_2Cl_2/Et_2O solution at room temperature. Anal. Calcd for $C_{24}H_{46}N_4Pt$ (MW 585.74): C, 49.21; H, 7.92; N, 9.57. Found: C, 49.32 ; H, 7.66 ; N, 9.60. ^{1}H NMR (C_6D_6, 400 MHz, δ): 7.28 (d, 1H, ^4J_H = 2.2; Hz, J^4_{Pt} = 7.2 Hz, C(2)-**H**), 6.82 (d, 1H, ^4J_H = 2.2; $^3J_{Pt}$ = 17.1 Hz, C(4)=C**H)** 6.77 (s, 2H, $^4J_{Pt}$ = 6.1 Hz C(4,5)=C**H**), 1.97 (s, 18H, C(C**H**$_3)_3$), 1.70 (s, 9H, C(C**H**$_3)_3$), 1.10 (s, 3H, $^2J_{Pt}$ = 67.0 Hz, C**H**$_3$), 0.89 (s, 3H, $^2J_{Pt}$ = 67.5 Hz, C**H**$_3$), 0.87 (s, 9H, C(C**H**$_3)_3$). ^{13}C NMR (THF-d_8, 400 MHz, δ): 191.8 (s, N-**C**-N), 165.2 (s, Pt-**C**=C), 125.9 (s, $^3J_{Pt}$ = 19.6 Hz, N-**C**(H)-N), 124.7 (s, $^3J_{Pt}$ = 59.4 Hz, **C**(H)=C-Pt), 117.4 (s, $^3J_{Pt}$ = 27.6 Hz, C(4,5)-*n*ItBu), 59.1 (s, N-**C**$(CH_3)_3$), 58.9 (s, N-**C**$(CH_3)_3$), 56.5 (s, N-**C**$(CH_3)_3$), 32.3 (s, C(**C**$H_3)_3$), 31.1 (s, C(**C**$H_3)_3$), 30.3 (s, C(**C**$H_3)_3$), -5.89 (s, $^1J_{Pt}$ = 604.2 Hz Pt-**C**H_3), -9.05 (s, $^1J_{Pt}$ = 616.2 Hz, Pt-**C**H_3).

Crystallographic Structure Determinations. Single-crystal x-ray diffraction data for *cis*-Pt(^{Me}Ime)$_2$Me$_2$ (**1**) were measured using an Enraf-Nonius Kappa CCD 4-circle diffractometer. Data for the remaining complexes (**2-7**) were measured using a Bruker SMART 1K CCD 3-circle diffractometer. The crystals were cooled and maintained at the data collection temperature using a stream of cold N_2 gas. Integrated intensities were calculated from the raw detector data using the program *SAINT*[6]. Empirical corrections for crystal absorption were calculated using the program *SADABS*[6], and the structures were solved and refined using *SHELX97*[7]. *cis*-Pt(ICy)$_2$Me$_2$, **2**, which crystallizes in the noncentrosymmetric space group, Cc, has a Flack[8] parameter of 0.021(5). For each complex, all hydrogen atoms were located in difference Fourier maps. However, independent refinement yielded unrealistic geometries of some of the hydrogen atoms due to the influence of the highly absorbing Pt atom. Therefore, hydrogen positions were constrained to idealized geometry using a model in which the hydrogen atoms ride on the atoms to which they are attached. However, for the (IMes)(IMes*)Pt(Me) complex, **5**, the hydrogen parameters on C42 were refined, since the constrained geometry may be inappropriate because of the C42-Pt1 interaction. To improve the initial convergence, 'rigid bond' restraints[9] on the anisotropic thermal displacement parameters were included in the refinements of complexes **2-7** with weighting factors of 0.007 Å^2. Refinement of the thermal displacement parameters of the N3 atom of complex **5** yielded values corresponding to a non-positive definite tensor. To correct this result, isotropic restraints on the thermal parameters on N3 were imposed with a weighting factor of 0.005 Å^2.

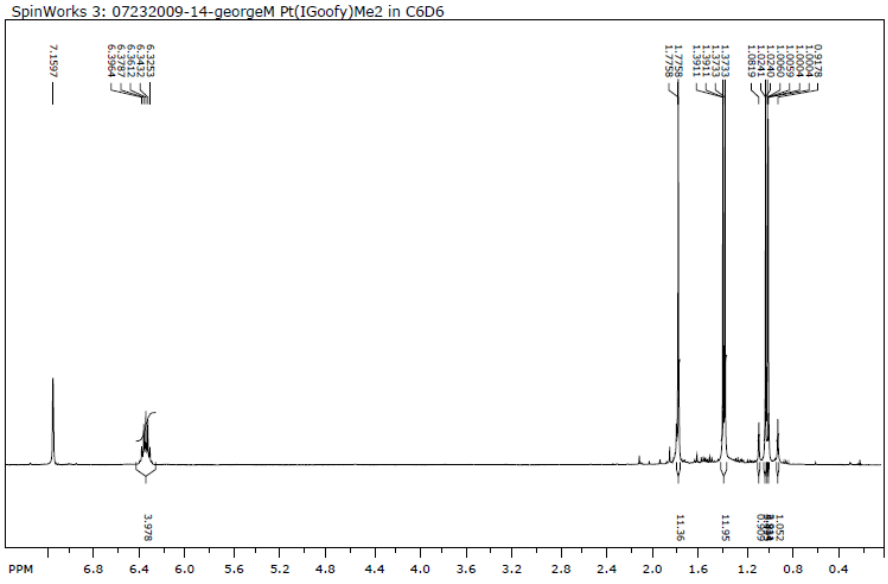
Table S1. Selected bond lengths and angles for complexes **1**-**7**

Complex	Pt–NHC	Pt–NHC	Pt–C	Pt–C
1	2.013(4)	2.027(5)	2.090(6)	2.117(5)
2	2.032(3)	2.065(3)	2.099(3)	2.107(3)
3	2.040(2)	2.053(2)	2.093(2)	2.095(2)
4	2.043(3)	2.044(3)	2.091(3)	2.093(3)
5	2.027(4)	2.053(4)[a]	2.105(4)[a]	2.096(4)
6	1.968(6)	1.985(6)	---	---
7	2.058(4)	2.074(4)[b]	2.079(4)	2.101(4)
Complex	NHC–Pt–NHC	NHC–Pt–C (*cis*)		C–Pt–C
1	92.8(2)	90.5(2), 91.2(2)		85.6(2)
2	94.0(1)	88.6(1), 93.3(1)		84.4(1)
3	96.7(1)	88.5(1), 90.6(1)		84.5(1)
4	113.0(1)	82.4(1), 83.6(1)		81.1(1)
5	108.4(2)	87.3(2), 79.8(2)[a]		84.3(2)[a]
6	178.3(2)	---		---
7	104.3(2)	84.9(2), 83.9(2)[b]		87.0(2)

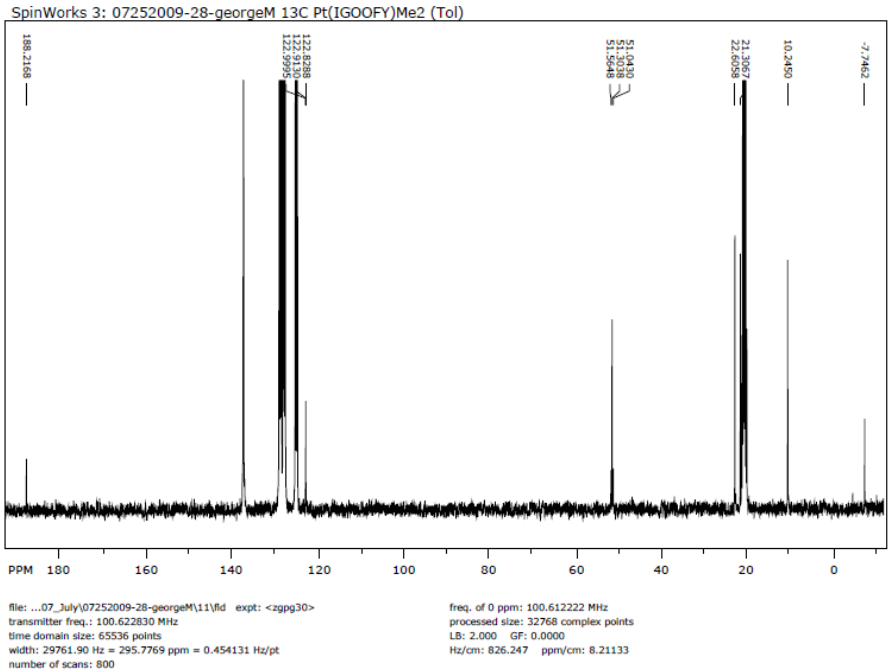
[a] Bond lengths and angles of cyclometallated IMes. [b] Bond lengths and angles of abnormally bound I^{t}Bu.

cis-Pt(^{Me}I^{i}Pr)$_2$Me$_2$ (3)

^{1}H NMR



^{13}C NMR



cis-Pt(^{Me}IMe)$_2$Me$_2$(1)

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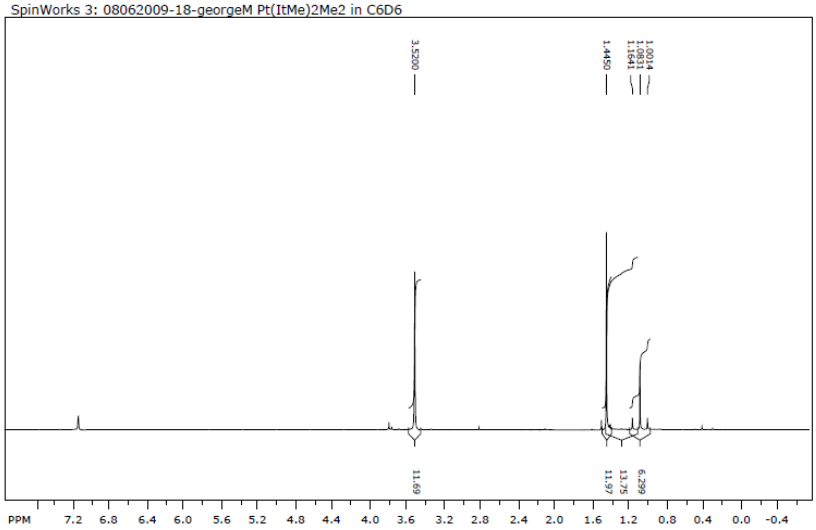

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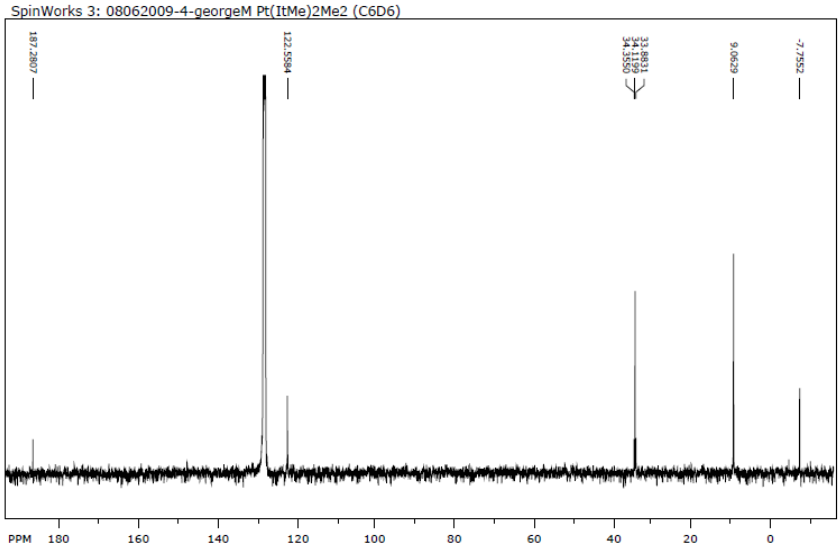

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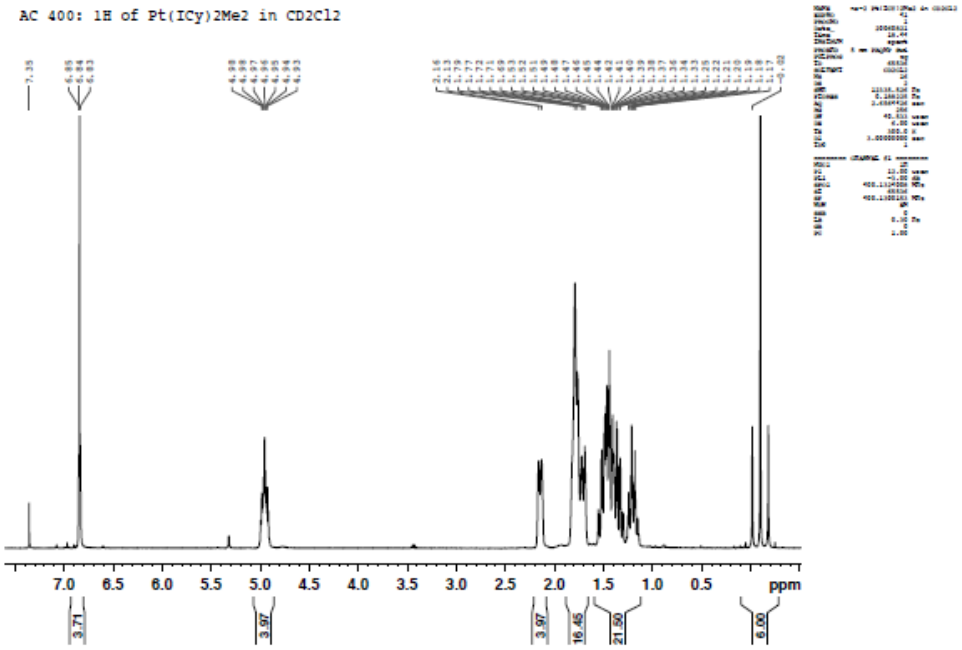
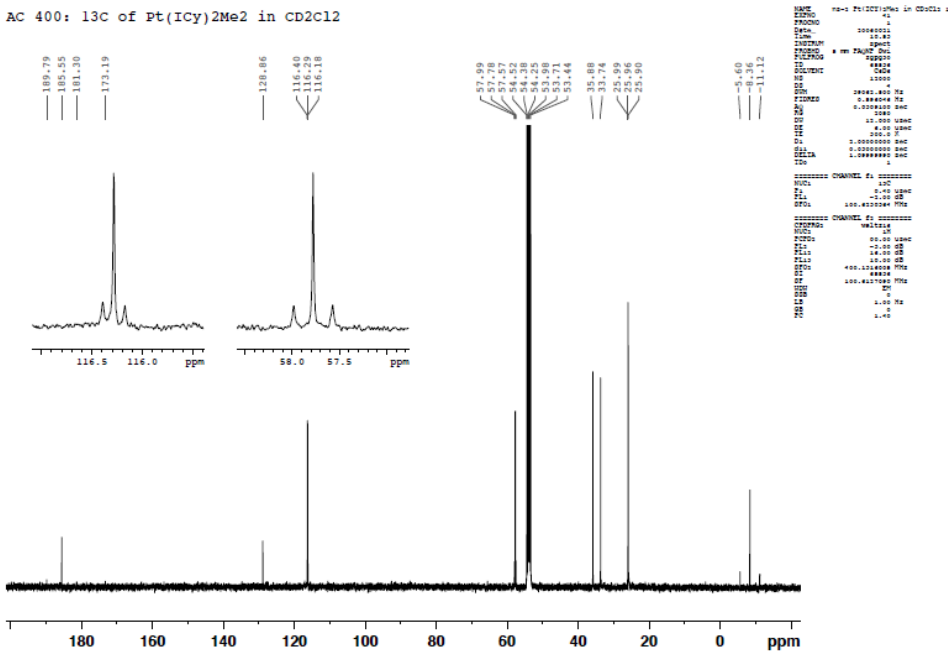
cis-Pt(ICy)$_2$Me$_2$ (2)

^{1}H NMR

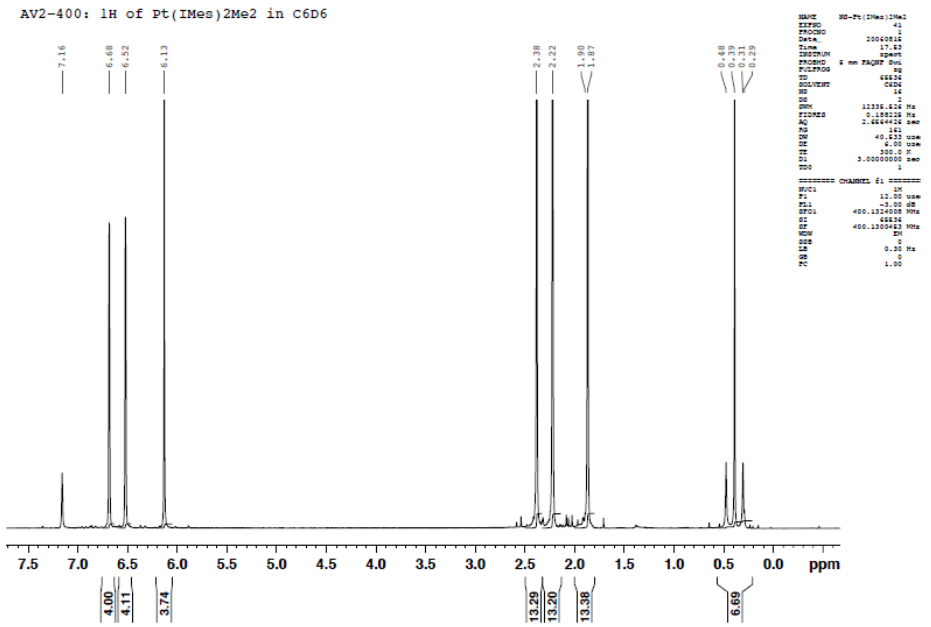


^{13}C NMR

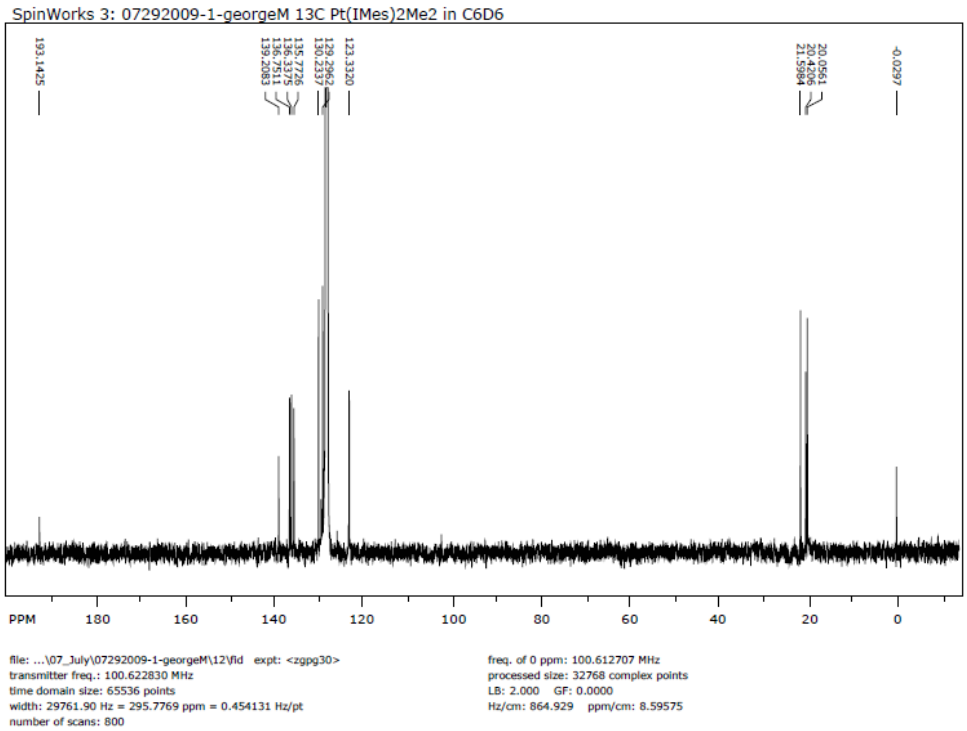


cis-Pt(IMes)$_2$Me$_2$ (4)

^{1}H NMR

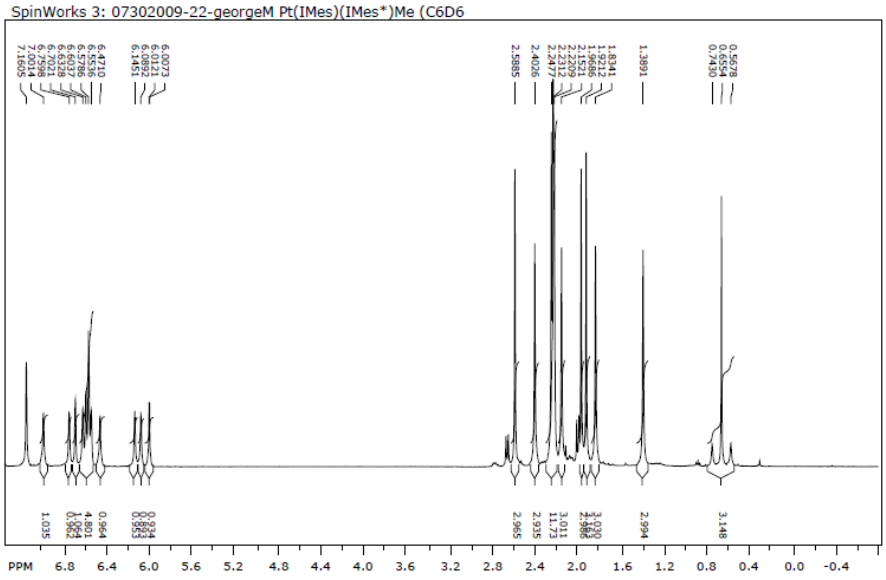


^{13}C NMR

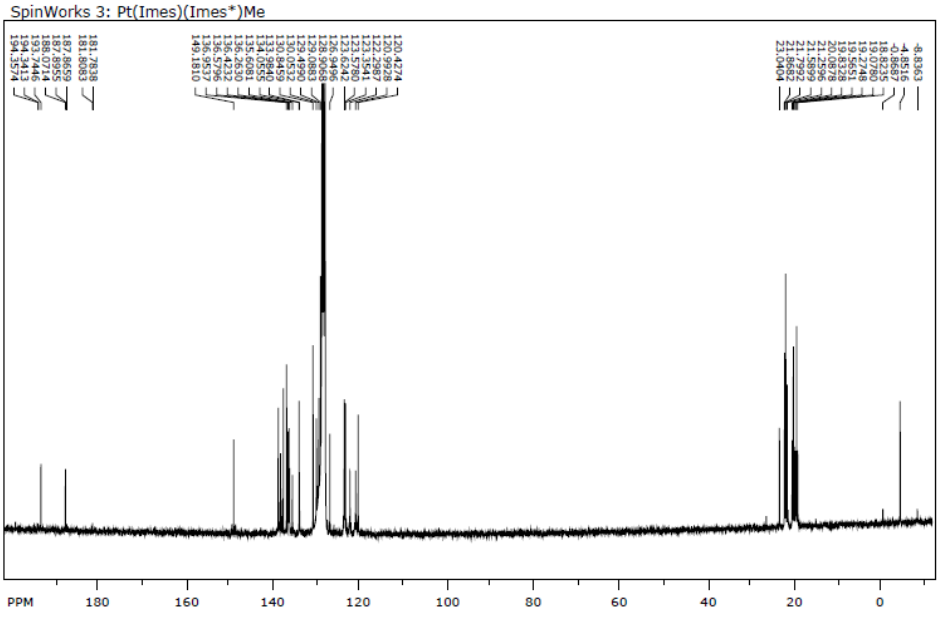


Pt(IMes)(IMes')Me (5)

^{1}H NMR

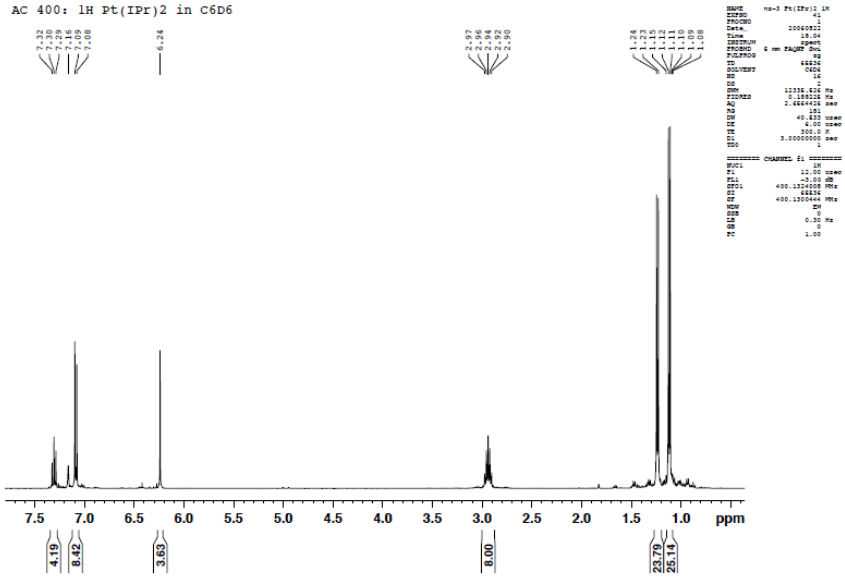


^{13}C NMR

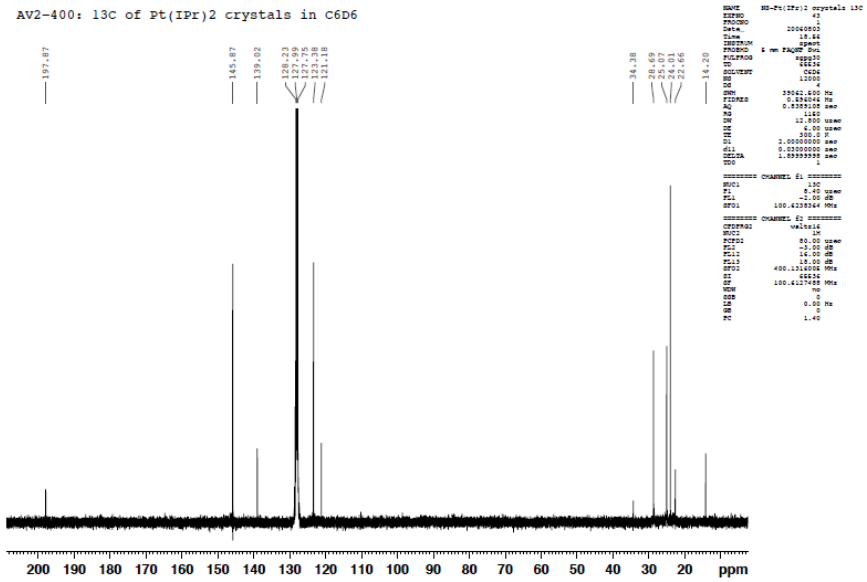


$Pt(IPr)_2$ (6)

^1H NMR

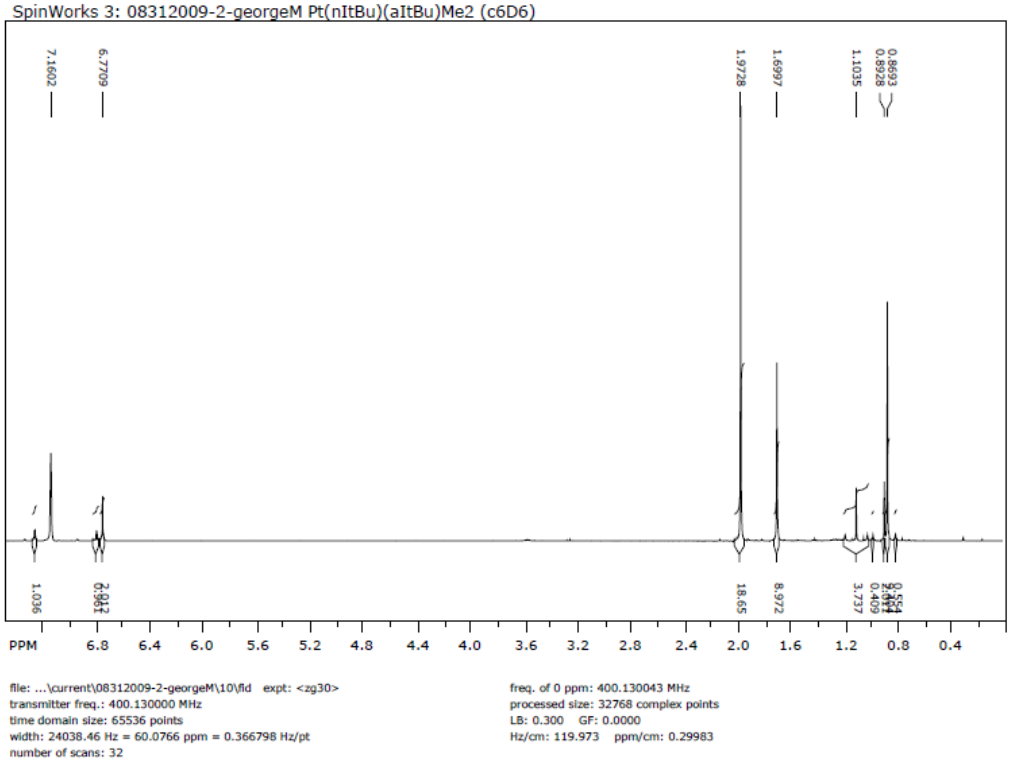


^{13}C NMR



Pt(*n*I^{t}Bu)(*a*I^{t}Bu)Me$_2$ (7)

^{1}H NMR



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number of scans: 32

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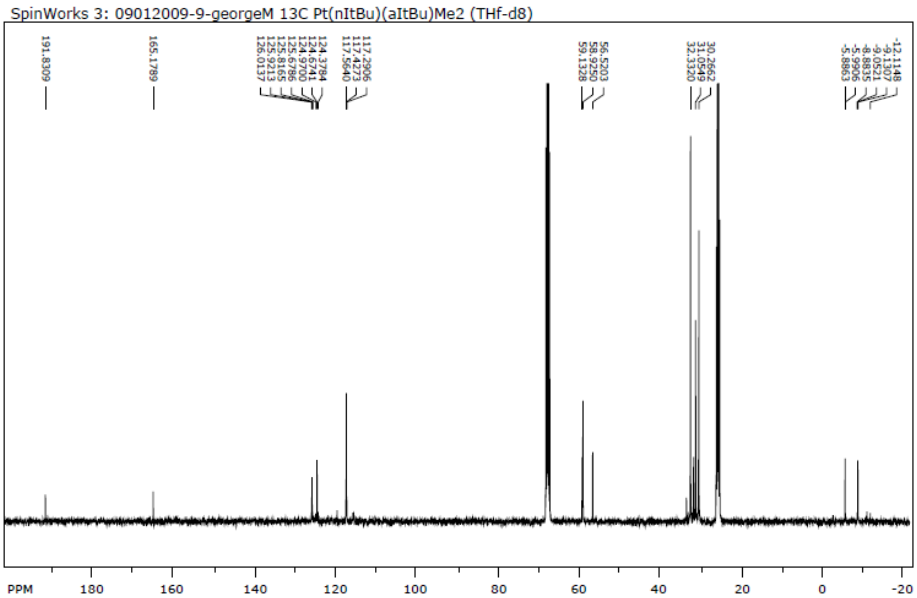
Hz/cm: 119.973 ppm/cm: 0.29983

^{13}C NMR



file: ...\current\09012009-9-georgeM\11\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 29761.90 Hz = 295.7769 ppm = 0.454131 Hz/pt
number of scans: 800

freq. of 0 ppm: 100.612648 MHz
processed size: 32768 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 900.763 ppm/cm: 8.95188

Burried volume of $^{Me}I^{i}Pr$ ligand:

SambVca@MoLNnaC

SambVca @ MoLNaC
Results page

```
 ---------------------------------------------------
|                                                   |
|                   S A M B V C A                   |
|                                                   |
|                Buried Volume in Salerno           |
|                                                   |
|     http://www.molnac.unisa.it/OM-tools/SambVca   |
|                                                   |
|     L. Cavallo et al. email: lcavallo@unisa.it    |
|                                                   |
 ---------------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/cfca9b5d4c5c4e16f5302ce5366fa247.c3d1

```
    Number of atoms              :   33
    Atom that is coordinated     :    1
    Atoms that define the axis   :    2
    ID of these atoms            :   32  33

    Radius of sphere (Angs)      :    3.500
    Distance from sphere (Angs)  :    2.020
    Mesh step (Angs)             :    0.050
    H atoms included in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C       3.48700    7.74700    1.77800
C       2.65400    9.86200    1.50900
C       3.99400    9.95900    1.57800
C       1.00600    7.88900    1.55400
C       0.09900    8.38500    2.67200
C       0.38300    8.05600    0.17200
C       5.90900    8.24400    1.80300
C       6.55800    8.35700    0.42600
C       6.69600    8.96500    2.88100
C       1.64300   10.96800    1.45500
C       4.82700   11.20700    1.56600
H      -0.21300    9.29000    2.46300
H      -0.67200    7.78500    2.75700
H       0.59600    8.39800    3.51600
H       1.00700    7.72800   -0.51000
H      -0.45000    7.54100    0.12500
H       0.19100    9.00300    0.01100
H       6.45900    9.27300    0.09200
H       7.51100    8.13500    0.49400
H       6.12200    7.73400   -0.19400
H       6.17700    8.97600    3.71200
H       7.54600    8.50100    3.03100
H       6.87300    9.88500    2.59500
H       2.08900   11.80700    1.21200
H       0.96000   10.75500    0.78600
H       1.22000   11.06700    2.33400
H       5.10800   11.42200    2.47900
H       5.61900   11.06400    1.00600
H       4.30000   11.94700    1.20200
H       1.16000    6.98200    1.71100
H       5.84100    7.37000    2.05000
N       2.35200    8.50100    1.62600
N       4.49100    8.66100    1.74600
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

```
H     1.29
CC    1.99
CB    1.99
C     1.99
NC    1.81
NB    1.81
N     1.81
O     1.78
F     1.72
P     2.11
Cl    2.05
```

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

```
C      -0.15721    2.00173   -0.22081
C      -0.99021    4.11673   -0.48981
C       0.34979    4.21373   -0.42081
C      -2.63821    2.14373   -0.44481
C      -3.54521    2.63973   -0.67319
C      -3.26121    2.31073   -1.82681
C       2.26479    2.49873   -0.19581
C       2.91379    2.61173   -1.57281
C       3.05179    3.21973   -0.88219
C      -2.00121    5.22273   -0.54381
C       1.18279    5.46173   -0.43281
H      -3.85721    3.54473   -0.46419
H      -4.31621    2.03973   -0.75819
H      -3.04821    2.65273   -1.51719
H      -2.63721    1.98273   -2.50881
H      -4.09421    1.79573   -1.87381
H      -3.45321    3.25773   -1.98781
H       2.81479    3.52773   -1.90681
H       3.86679    2.38973   -1.50481
H       2.47779    1.98873   -2.19281
H       2.53279    3.23073   -1.71319
H       3.90179    2.75573   -1.03219
H       3.22879    4.13973   -0.59619
H      -1.55521    6.06173   -0.78681
H      -2.68421    5.00973   -1.21281
H      -2.42421    5.32173   -0.33519
H       1.46379    5.67673   -0.48019
H       1.97479    5.31873   -0.99281
H       0.65579    6.20173   -0.79681
H      -2.48421    1.23673   -0.28781
H       2.19679    1.62473   -0.05119
N      -1.29221    2.75573   -0.37281
N       0.84679    2.91573   -0.25281
XX      0.00000    0.00000    0.00000
```

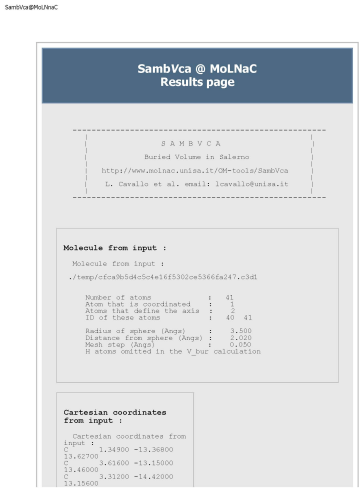
Results : Volumes in Angs^3

Results : Volumes in Angs^3

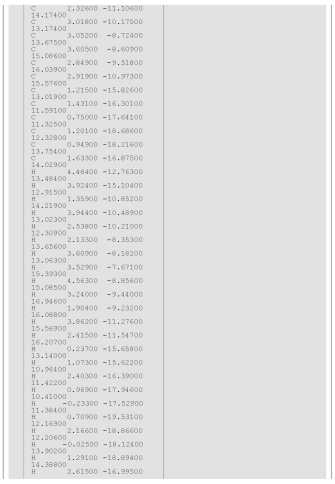
```
      N of voxels examined :        1436277
      Volume of voxel      :      0.125E-03

  V Free   V Buried  V Total   V Exact
 129.415    50.119   179.535   179.594

 %V Free   %V Bur   % Tot/Ex
  72.084    27.916    99.967
```

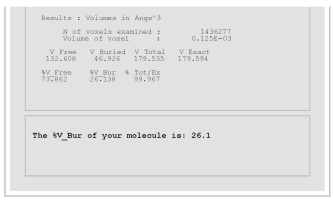
The %V_Bur of your molecule is: 27.9

Burried volume of ICy ligand:

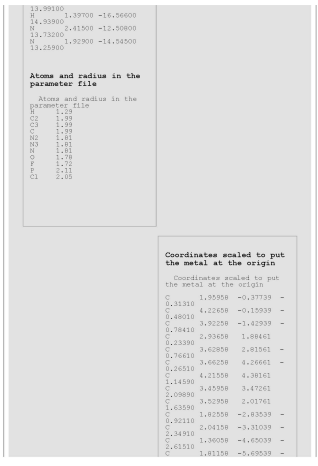


file:///C|/...ttings/George%20Fortman/Desktop/Nolan/(NCH)2PMe2/Xray/Vburn/Equadistance/Pt(ICy)2Me2%20with%20H.htm[7/21/2009 1:04:45 PM]





file:///C|/...ttings/George%20Fortman/Desktop/Nolan/(NCH)2PMe2/Xray/Vburn/Equadistance/Pt(ICy)2Me2%20with%20H.htm(7/21/2009 1:04:45 PM)



file:///C|/...ttings/George%20Fortman/Desktop/Nolan/(NCH)2PMe2/Xray/Vburn/Equadistance/Pt(ICy)2Me2%20with%20H.htm[7/21/2009 1:04:45 PM]

Burried volume of IMes ligand:

SambVca@MoLNaC

SambVca @ MoLNaC
Results page

S A M B V C A
Buried Volume in Salerno
http://www.molnac.unisa.it/OM=tools/SambVca
L. Cavallo et al. email: lcavallo@unisa.it

Molecule from input :

Molecule from input :
./temp/cfca9b5dd5c5c4e16f5302ce5366fa247.c3d1

Number of atoms : 47
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 46 47

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.020
Mesh step (Angs) : 0.050
H atoms included in the V_bur calculation

Cartesian coordinates from input :

Cartesian coordinates from input :

C	-4.73500	3.24900	
2.14300			
C	-4.25300	2.14300	
4.09200			
C	-5.57600	2.27700	
4.04100			

SambVca@MoLNaC

2.39249			
C	4.51875	-0.89936	
2.47349			
C	3.14975	-0.60936	
2.42149			
C	2.67675	0.80864	
2.52549			
C	4.48075	-2.45936	
2.57349			
C	1.79475	-4.17536	
1.98449			
C	-2.64825	-1.13136	
2.01249			
C	-3.08125	-2.00736	
1.01849			
C	-4.42225	-1.96536	
0.64949			
C	-5.31625	-1.08736	
1.25749			
C	-4.84025	-0.23336	
2.22949			
C	-3.50925	-0.25036	
2.64949			
C	-3.08525	0.63364	
3.79649			
C	-5.77625	-1.08336	
0.86649			
C	-2.13425	-2.98836	
0.38349			
H	0.82775	-2.49536	
4.40649			
H	-1.62025	-2.25536	
4.30549			
H	4.42975	-4.10536	
2.06749			
H	3.13475	-0.18336	
2.57049			
H	1.93975	0.86164	
3.16849			
H	3.41575	1.37764	
2.82749			
H	2.36575	1.11564	
1.64749			
H	6.63775	-2.82236	
3.46949			
H	6.77875	-3.10836	
1.90149			
H	6.98175	-1.62436	
2.46549			
H	1.48775	-4.47336	
2.86549			
H	1.02175	-3.90736	
1.44349			
H	2.26775	-4.90836	
1.53749			
H	-4.73625	-2.54936	-
0.03151			
N	-5.44025	0.38664	
2.62749			
C	-7.11125	0.73064	
3.79149			
H	-1.50225	1.51664	
3.69949			
H	-3.36925	0.23064	
4.64249			
H	-7.27925	-0.52336	
1.49249			
H	-6.87025	-0.72436	-
0.04051			

SambVca@MoLNaC

C	-2.31500	2.54500	
2.68800			
C	-1.85400	1.23100	
2.53000			
C	-0.47900	1.00800	
2.56900			
C	0.42500	2.04000	
2.77600			
C	-0.06300	3.33000	
2.85700			
C	-1.43200	3.62000	
2.80500			
C	-1.90500	5.03800	
2.90900			
O	1.89900	1.77000	
2.95700			
C	-2.78700	0.05400	
2.36800			
C	-7.22600	3.09800	
2.39600			
C	-7.66300	2.22200	
1.40200			
C	-9.00400	2.26400	
1.03300			
C	-9.89800	3.14200	
1.64100			
C	-9.42200	3.99600	
2.61300			
C	-8.08100	3.97900	
3.03300			
C	-7.66700	4.86300	
4.18000			
C	-11.35800	3.14600	
1.25000			
C	-6.71600	1.24100	
0.76700			
N	-3.75400	1.73400	
4.79000			
H	-6.28200	1.97400	
4.68900			
H	-0.15200	0.12400	
2.45100			
N	0.55300	4.04600	
2.95400			
H	-2.64200	5.09100	
3.55200			
N	-1.16600	5.60700	
2.21100			
N	-2.21600	5.34500	
2.03100			
H	2.05600	1.40700	
3.85300			
H	2.19700	1.12100	
2.28500			
H	2.40000	2.40500	
2.84900			
H	-3.09400	-0.24480	
3.24900			
H	-3.56000	0.32200	
1.82700			
H	-2.31400	-0.67900	
1.92100			
H	-9.31800	1.68000	
0.35200			
H	-10.02200	4.61600	
3.01100			
H	-6.69300	4.96000	
4.17500			
H	-8.08400	5.74600	

SambVca@MoLNaC

H	-7.12325	-1.99836	
0.89449			
H	-1.70825	-3.52936	
1.08149			
H	-2.63025	-3.57336	-
0.22651			
H	-1.44725	-2.50036	-
0.11751			
N	0.84775	-1.51436	
2.54549			
N	-1.28525	-1.28436	
2.47749			
Xe	0.00000	0.00000	
0.00000			

Results : Volumes in Angs^3

Results : Volumes in Angs^3

N of voxels examined :	1436277
Volume of voxel :	0.125E-03

V_Free	V_Buried	V_Total	V_Exact
118.189	61.345	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
65.831	34.169	99.967

The %V_Bur of your molecule is: 34.2

SambVca@MoLNaC

H	-7.95100	4.46000	
4.08300			
H	-11.86100	3.70600	
5.02600			
H	-11.45200	3.50500	
1.87600			
H	-11.70500	2.23100	
0.34300			
I	-6.29000	0.70000	
3.27800			
N	-7.21200	0.65600	
3.46500			
H	-6.02900	1.72900	
0.33700			
H	-3.73400	2.71500	
0.26600			
N	-5.86700	2.94500	
2.92900			
N			
2.46100			

Atoms and radius in the parameter file

Atoms and radius in the parameter file

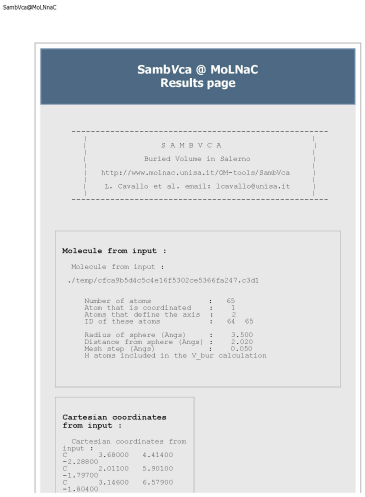
H	1.29
C2	1.99
C3	1.99
C	1.99
N2	1.81
N3	1.81
N	1.81
O	1.78
P	2.11
Pt	2.13
Cl	2.05

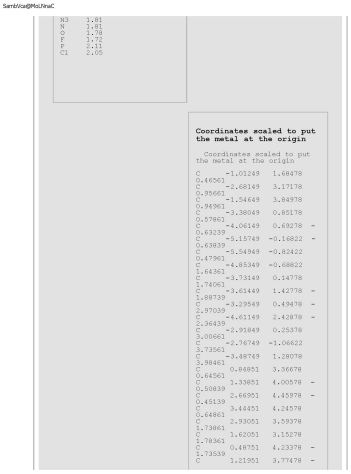
Coordinates scaled to put the metal at the origin

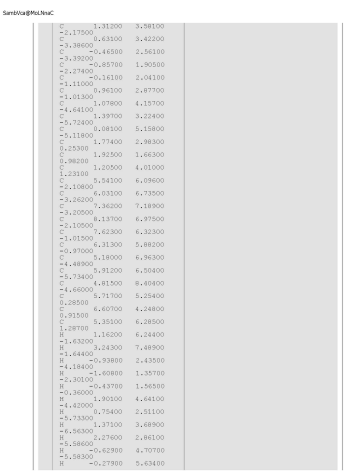
Coordinates scaled to put the metal at the origin

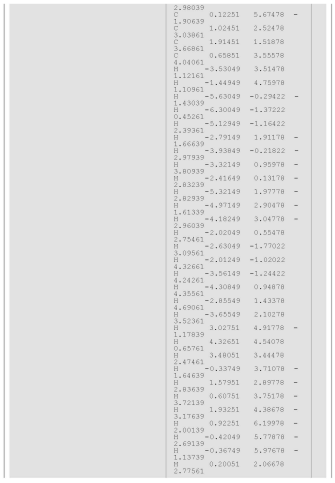
C	-0.15325	-0.98036	
1.75949			
C	0.32675	-2.08636	
3.70949			
C	-0.99425	-1.95236	
2.65749			
C	2.26675	-1.68436	
2.90449			
C	2.72775	-2.99036	
2.14649			
C	4.10275	-3.22136	
2.18549			
C	5.00675	-2.18936	

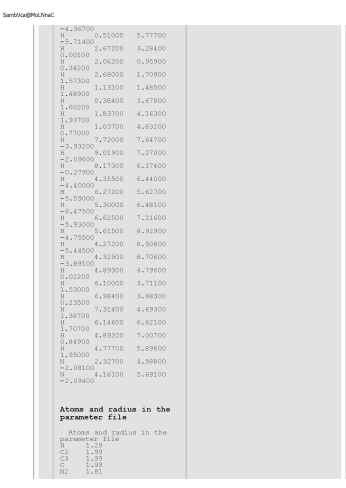
Burried volume of IPr ligand:











Burried volume of *n*I^{t}Bu ligand:

SambVca@MoLNinaC

SambVca @ MoLNaC
Results page

```
 ---------------------------------------------------
|                                                   |
|                  S A M B V C A                    |
|                                                   |
|               Buried Volume in Salerno            |
|                                                   |
|    http://www.molnac.unisa.it/OM-tools/SambVca    |
|                                                   |
|    L. Cavallo et al. email: lcavallo@unisa.it     |
|                                                   |
 ---------------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/cfca9b5d4c5c4e16f5302ce5366fa247.c3d1

```
    Number of atoms              :   33
    Atom that is coordinated     :    1
    Atoms that define the axis   :    2
    ID of these atoms            :   32  33

    Radius of sphere (Angs)      :    3.500
    Distance from sphere (Angs)  :    2.020
    Mesh step (Angs)             :    0.050
    H atoms included in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C       8.73100   13.72600   -2.77600
C       7.36900   15.49300   -3.29100
C       8.63400   15.95100   -3.32000
```

SambVca@MoLNinaC

```
H       1.29
C2      1.99
C3      1.99
C       1.99
N2      1.81
N3      1.81
N       1.81
O       1.78
P       1.72
Cl      2.05
```

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

```
C      -0.68465    1.83830   -0.48197
C      -2.04665    3.60530   -0.99697
C      -0.78165    4.06330   -1.02597
C       1.52635    3.16430   -0.50297
C       1.96535    4.50930   -1.09697
C       1.78935    3.17030   -1.00903
C       2.30735    2.05830   -1.21997
C      -3.30665    1.51730   -0.56697
C      -3.17365    0.08030   -0.08597
C      -3.97565    1.54630   -1.95397
C      -4.18165    2.26430   -0.44503
H      -2.83065    4.11030   -1.17297
H      -0.50465    4.95030   -1.22297
H       1.57435    5.24030   -0.57297
H       2.94235    4.57530   -1.07097
H       1.65935    4.57230   -2.02497
H       1.51135    2.31230   -1.39303
H       2.74535    3.30730   -1.17403
H       1.27735    3.89530   -1.42603
H       2.10135    2.08130   -2.17797
```


file:///C|/...tings/George%20Fortman/Desktop/Nolan/(NCH)2PtMe2/Xray/Vburr/Equadistance/Pt(tBu)2Me2%20with%20H.htm[7/21/2009 1:04:46 PM]

SambVca@MoLNinaC

```
C      10.94200   15.05200   -2.79700
C      11.38100   16.39700   -3.39100
C      11.20500   15.05800   -1.28500
C      11.72300   13.94600   -3.51400
C       6.10900   13.40500   -2.86100
C       6.24200   11.96800   -2.38000
C       5.44000   13.43400   -4.24800
C       5.23400   14.15200   -1.84900
H       6.58500   15.99800   -3.46700
H       8.91100   16.83800   -3.51700
H      10.99000   17.12800   -2.86700
H      12.35800   16.46300   -3.36500
H      11.07500   16.46000   -4.31900
H      10.92700   14.20000   -0.90100
H      12.16100   15.19500   -1.12000
H      10.69300   15.78300   -0.86800
H      11.51700   13.96900   -4.47200
H      12.68400   14.08700   -3.38300
H      11.46700   13.07400   -3.14600
H       6.60700   11.96000   -1.47000
H       5.36100   11.53900   -2.38300
H       6.84500   11.47800   -2.97700
H       6.00500   12.95800   -4.89200
H       4.56400   12.99800   -4.19800
H       5.32700   14.36400   -4.53700
H       5.12900   15.08500   -2.13200
H       4.35200   13.72500   -1.80000
H       5.65900   14.12500   -0.96600
N       9.46300   14.87100   -3.00700
N       7.41800   14.14100   -2.95400
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

SambVca@MoLNinaC

```
H       3.26835    2.19930   -1.08897
H       2.05135    1.18630   -0.85197
H      -2.80865    0.07230   -0.82403
H      -4.05465   -0.34870   -0.08897
H      -2.57065   -0.40970   -0.68297
H      -3.41065    1.07030   -2.59797
H      -4.85165    1.11030   -1.90397
H      -4.08865    2.47630   -2.24297
H      -4.28665    3.19730   -0.16203
H      -5.06365    1.83730   -0.49403
H      -3.75665    2.23730   -1.32803
N       0.04735    2.98330   -0.71297
N      -1.99765    2.25330   -0.65997
XX      0.00000    0.00000    0.00000
```

Results : Volumes in Angs^3

Results : Volumes in Angs^3

```
     N of voxels examined :        1436277
     Volume of voxel      :      0.125E-03

  V Free   V Buried  V Total   V Exact
 113.085    66.449   179.535   179.594

 %V_Free    %V_Bur  % Tot/Ex
 62.988     37.012    99.967
```

The %V_Bur of your molecule is: 37.0

file:///C|/...tings/George%20Fortman/Desktop/Nolan/(NCH)2PtMe2/Xray/Vburr/Equadistance/Pt(tBu)2Me2%20with%20H.htm[7/21/2009 1:04:46 PM]
file:///C|/...tings/George%20Fortman/Desktop/Nolan/(NCH)2PtMe2/Xray/Vburr/Equadistance/Pt(tBu)2Me2%20with%20H.htm[7/21/2009 1:04:46 PM]

Burried volume of ^{Me}IMe:

SambVca@MoLNnaC

SambVca @ MoLNaC
Results page

```
   ------------------------------------------------------
   |                                                    |
   |                  S A M B V C A                     |
   |                                                    |
   |              Buried Volume in Salerno              |
   |                                                    |
   |    http://www.molnac.unisa.it/OM-tools/SambVca     |
   |                                                    |
   |     L. Cavallo et al. email: lcavallo@unisa.it     |
   |                                                    |
   ------------------------------------------------------
```

Molecule from input :

```
 Molecule from input :

./temp/cfca9b5d4c5c4e16f5302ce5366fa247.c3d1


    Number of atoms            :   21
    Atom that is coordinated   :    1
    Atoms that define the axis :    2
    ID of these atoms          :   20  21

    Radius of sphere (Angs)    :    3.500
    Distance from sphere (Angs) :   2.100
    Mesh step (Angs)           :    0.050
    H atoms included in the V_bur calculation
```

Cartesian coordinates from input :

```
  Cartesian coordinates from input :
C        5.27200    1.96000    4.31300
C        6.16600    4.07200    4.39000
C        4.83200    4.20200    4.17100
C        7.71100    2.10900    4.64500
C        7.24000    5.09700    4.49900
C        3.95400    5.40900    4.04300
C        2.91500    2.59300    3.85900
H        8.29300    2.36900    3.90200
H        8.10200    2.41500    5.49100
H        7.61900    1.13200    4.66300
H        6.83600    5.98900    4.54400
H        7.76600    4.93500    5.31000
H        7.82400    5.04300    3.71400
H        4.49100    6.21800    4.17100
H        3.54700    5.42300    3.15100
H        3.24900    5.37500    4.72200
H        2.80200    1.62100    3.81900
H        2.36000    2.95700    4.58100
H        2.64100    2.99000    3.00600
N        6.41800    2.70700    4.47400
N        4.32000    2.91200    4.11700
```

Atoms and radius in the parameter file

```
  Atoms and radius in the parameter file
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
F     1.72
P     2.11
Cl    2.05
```

Coordinates scaled to put the metal at the origin

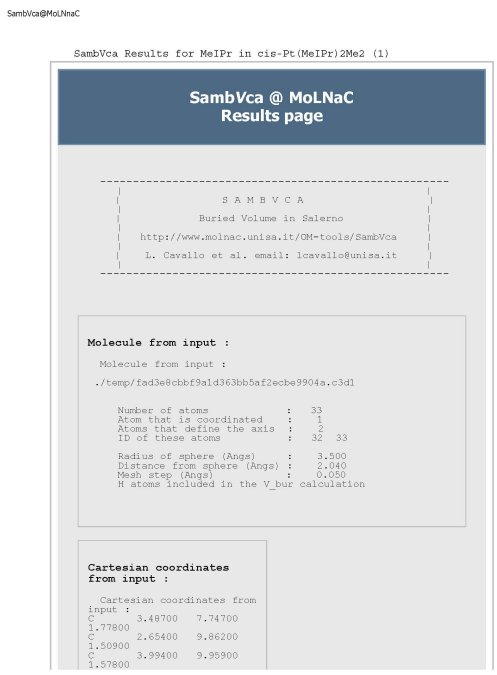
```
  Coordinates scaled to put the metal at the origin
C        0.23819    2.08601   -0.04297
C        1.13219    4.19801   -0.03403
C       -0.20181    4.32801   -0.18497
C        2.67719    2.23501   -0.28903
C        2.20619    5.22301   -0.14303
C       -1.07981    5.53501   -0.31297
C       -2.11881    2.71901   -0.49697
H        3.25919    2.49501   -0.45397
H        3.06819    2.54101   -1.13503
H        2.58519    1.25801   -0.30703
H        1.80219    6.11501   -0.18803
H        2.73219    5.06101   -0.95403
H        2.79019    5.16901   -0.64197
H       -0.54281    6.34401   -0.18497
H       -1.48681    5.54901   -1.20497
H       -1.78481    5.50101   -0.36603
H       -2.23181    1.74701   -0.53697
H       -2.67381    3.08301   -0.22503
H       -2.39281    3.11601   -1.34997
H        1.38419    2.83301   -0.11803
N       -0.71381    3.03801   -0.23897
XX       0.00000    0.00000    0.00000
```

Results : Volumes in Angs^3

```
  Results : Volumes in Angs^3

      N of voxels examined :         1436277
      Volume of voxel      :       0.125E-03

   V Free    V Buried  V Total   V Exact
  133.833     45.702   179.535   179.594

  %V_Free     %V_Bur   % Tot/Ex
   74.544     25.456    99.967
```

The %V_Bur of your molecule is: 25.5

Burried volume of *a*l^{t}Bu ligand:


SambVca@MoLNnaC

SambVca Results for MeIPr in cis-Pt(MeIPr)2Me2 (1)

SambVca @ MoLNaC
Results page

S A M B V C A
Buried Volume in Salerno
http://www.molnac.unisa.it/OM-tools/SambVca
L. Cavallo et al. email: lcavallo@unisa.it

Molecule from input :

Molecule from input :

./temp/fad3e8cbbf9a1d363bb5af2ecbe9904a.c3d1

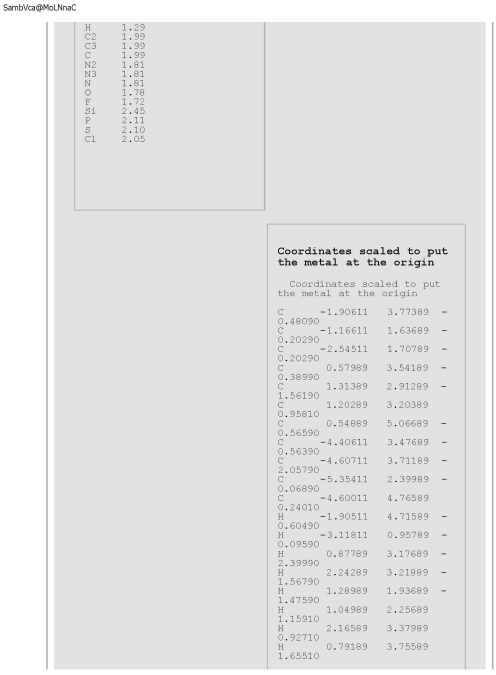
Number of atoms : 33
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 32 33

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.040
Mesh step (Angs) : 0.050
H atoms included in the V_bur calculation

Cartesian coordinates from input :

Cartesian coordinates from input :

C 3.48700 7.74700 1.77800
C 2.65400 9.86200 1.50900
C 3.99400 9.95900 1.57800

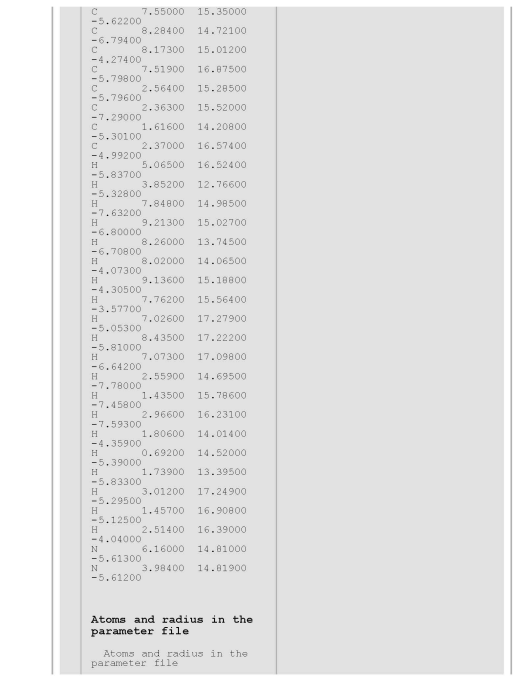

SambVca@MoLNnaC

H 1.29
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.76
F 1.72
Si 2.45
P 2.11
S 2.10
Cl 2.05

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

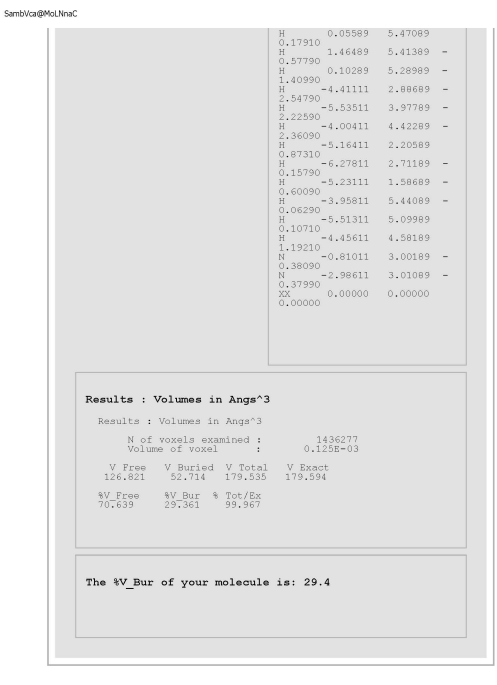
C -1.90611 3.77389 -0.48090
C -1.16611 1.63689 -0.20290
C -2.54511 1.70789 -0.20290
C 0.57989 3.54189 -0.38990
C 1.31389 2.91289 -1.56190
C 1.20289 3.20389 0.95810
C 0.54889 5.06689 -0.56590
C -4.40611 3.47689 -0.56390
C -4.60711 3.71189 -2.05790
C -5.35411 2.39989 -0.06890
C -4.60011 4.76589 0.24010
H -1.90511 4.71589 -0.60490
H -3.11811 0.95789 -0.09590
H 0.87789 3.17689 -2.39990
H 2.24289 3.21889 -1.56790
H 1.28989 1.93689 -1.47590
H 1.04989 2.25689 1.15910
H 2.16589 3.37989 0.92710
H 0.79189 3.75589 1.65510


SambVca@MoLNnaC

C 7.55000 15.35000 -5.62200
C 8.28400 14.72100 -6.79400
C 8.17300 15.01200 -4.27400
C 7.51900 16.87500 -5.79800
C 2.56400 15.28500 -5.79600
C 2.36300 15.52000 -7.29000
C 1.61600 14.20800 -5.30100
C 2.37000 16.57400 -4.99200
H 5.06500 16.52400 -5.83700
H 3.85200 12.76600 -5.32800
H 7.84800 14.98500 -7.63200
H 9.21300 15.02700 -6.80000
H 8.26000 13.74500 -6.70800
H 8.02000 14.06500 -4.07300
H 9.13600 15.18800 -4.30500
H 7.76200 15.56400 -3.57700
H 7.02600 17.27900 -5.05300
H 8.43500 17.22200 -5.81000
H 7.07300 17.09800 -6.64200
H 2.55900 14.69500 -7.78000
H 1.43500 15.78600 -7.45800
H 2.96600 16.23100 -7.59300
H 1.80600 14.01400 -4.35900
H 0.69200 14.52000 -5.39000
H 1.73900 13.39500 -5.83300
H 3.01200 17.24900 -5.29500
H 1.45700 16.90800 -5.12500
H 2.51400 16.39000 -4.04000
N 6.16000 14.81000 -5.61300
N 3.98400 14.81900 -5.61200

Atoms and radius in the parameter file

Atoms and radius in the parameter file


SambVca@MoLNnaC

H 0.05589 5.47089 0.17910
H 1.46489 5.41389 -0.57790
H 0.10289 5.28989 -1.40990
H -4.41111 2.88689 -2.54790
H -5.53511 3.97789 -2.22590
H -4.00411 4.42289 -2.36090
H -5.16411 2.20589 0.87310
H -6.27811 2.71189 -0.15790
H -5.23111 1.58689 -0.60090
H -3.95811 5.44089 -0.06290
H -5.51311 5.09989 0.10710
H -4.45611 4.58189 1.19210
N -0.81011 3.00189 -0.38090
N -2.98611 3.01089 -0.37990
XX 0.00000 0.00000 0.00000

Results : Volumes in Angs^3

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
126.821	52.714	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
70.639	29.361	99.967

The %V_Bur of your molecule is: 29.4

References:

[1] N. Kuhn, T. Kratz, *Synthesis* **1993**, *1993*, 561.
[2] A. J. Arduengo, R. Krafczyk, R. Schmutzler, H. A. Craig, J. R. Goerlich, W. J. Marshall, M. Unverzagt, *Tetrahedron* **1999**, *55*, 14523.
[3] L. Jafarpour, E. D. Stevens, S. P. Nolan, *Journal of Organometallic Chemistry* **2000**, *606*, 49.
[4] N. M. Scott, R. Dorta, E. D. Stevens, A. Correa, L. Cavallo, S. P. Nolan, *Journal of the American Chemical Society* **2005**, *127*, 3516.
[5] Reactivity of IMes depends on the source of Platinum-dimethyl precursor used. Reactions run with non-commercial (COD)Pt(Me)$_2$ gave faster conversion of complex **4** to **5**. More detailed discussion and possible causes are now being investigated.
[6] *SAINT* and *SADABS*, **2007**, Bruker AXS Inc., Madison, Wisconsin, USA.
[7] *SHELX97*, G. M. Sheldrick, *Acta Crystallogr. Sect. A*, **2008**, *64*, 112-122.
[8] H. D. Flack, *Acta Crystallogr. Sect. A*, **1983**, *39*, 876-881.
[9] F. L. Hirshfeld, *Acta Crystallogr. Sect. A*, **1976**, *32*, 239-244.

Table S2. Summary of crystallographic data for complexes **1-7**

Complex	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Chemical Formula	$C_{16}H_{30}N_4Pt$	$C_{32}H_{54}N_4Pt + CH_2Cl_2$	$C_{24}H_{46}N_4Pt$	$C_{44}H_{54}N_4Pt$	$C_{43}H_{50}N_4Pt$	$C_{54}H_{72}N_4Pt$	$C_{24}H_{46}N_4Pt$
Formula Weight (M)	473.44	774.81	585.74	834.00	817.96	972.25	585.74
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Unit-cell dimensions, V_{cell}	a=14.8926(2) Å b=8.1788(1) Å c=16.1119(2) Å β=113.5403(8)° V= 1799.17(4)Å^3	a=15.5185(7) Å b=12.9037(2) Å c=17.4636(8) Å β=105.354(1)° V= 3372.2(3) Å^3	a=15.9482(6) Å b=9.6101(3) Å c=17.6283(6) Å β=105.619(1)° V= 2601.0(2) Å^3	a=16.7156(10) Å b=13.1785(8) Å c=17.6422(10) Å β=99.411(1)° V= 3834.0(4) Å^3	a=10.7787(5) Å b=20.0707(9) Å c=17.2875(8) Å β=91.064(1)° V= 3739.3(3) Å^3	a=12.8035(7) Å b=26.9007(16) Å c=14.1517(8) Å β=92.184(1)° V= 4870.6(5) Å^3	a=12.0260(9) Å b=14.6685(11) Å c=14.7642(10) Å β=91.103(1)° V= 2604.0(3) Å^3
Temperature	160(1) K	150(2) K	150(2) K	150(2) K	150(2) K	150(2) K	173(2)
Space group	$P2_1/n$	Cc	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
Formula units/unit cell (Z)	4	4	4	4	4	4	4
N_{ref} (measured)	50417	27974	41062	40209	53108	63794	31831
N_{ref} (independent)	5253	10221	7606	11107	9017	10593	6239
R_{int}	0.0753	0.0195	0.0336	0.0373	0.0706	0.0478	0.0706
$2\theta_{max}$	60.0	61.0	60.0	60.0	56.0	54.0	56.0
R_{F^2}	0.0439	0.0252	0.0223	0.0420	0.0548	0.0584	0.0584
R_{F^2} ($I > 2\sigma_I$)	0.0375	0.0196	0.0187	0.0312	0.0422	0.0475	0.0325
CCDC no.	741809	741810	741808	741811	741812	741813	756172