Table 3. Selected bond lengths [Å] and angles [°] for SBH01.

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Plane dihedral angle
Plane 1 – Plane 2 4.83(5)

Deviation within planes

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Table 4. Bond lengths [Å] and angles [°] for SBH01.

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Table 5. Anisotropic displacement parameters (Å² x 10⁴) for SBH01. The anisotropic displacement factor exponent takes the form: -2π² [ h² a*²U₁₁ + ... + 2 h k a* b* U₁₂ ]

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Table 6. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^{-3}$) for SBH01.

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<td>5440(20)</td>
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<td>8139(19)</td>
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Crystal Structure Analysis of:

(BQA)NiCl (9) - SBH05

Contents

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Table 3. Selected bond distances and angles
Table 4. Full bond distances and angles (for deposit)
Table 5. Anisotropic displacement parameters
Table 6. Hydrogen atomic coordinates
Table 7. Observed and calculated structure factors (for deposit)
Table 1. Crystal data and structure refinement for SBH05.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tr>
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<td>Formula weight</td>
<td>364.47</td>
</tr>
<tr>
<td>Crystallization Solvent</td>
<td>Chloroform/hexanes</td>
</tr>
<tr>
<td>Crystal Habit</td>
<td>Block</td>
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<tr>
<td>Crystal size</td>
<td>0.23 x 0.20 x 0.20 mm(^3)</td>
</tr>
<tr>
<td>Crystal color</td>
<td>Dark red</td>
</tr>
<tr>
<td>Preliminary Photos</td>
<td>Rotation</td>
</tr>
<tr>
<td>Type of diffractometer</td>
<td>CCD area detector</td>
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<tr>
<td>Wavelength</td>
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<tr>
<td>Unit cell dimensions</td>
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<tr>
<td></td>
<td>(b = 11.4785(9)) Å</td>
</tr>
<tr>
<td></td>
<td>(c = 14.9909(12)) Å</td>
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<tr>
<td></td>
<td>(\beta = 107.3220(10)) (^\circ)</td>
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<td>Volume</td>
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<td>(Z)</td>
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<td>Density (calculated)</td>
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<tr>
<td>Independent reflections</td>
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<tr>
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<td>Absorption correction</td>
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### Table 1 (cont.)

**Structure solution and Refinement**

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<td>Patterson method</td>
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<tr>
<td>Secondary solution method</td>
<td>Difference Fourier map</td>
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<td>Hydrogen placement</td>
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<tr>
<td>Treatment of hydrogen atoms</td>
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<td>Goodness-of-fit on $F^2$</td>
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<tr>
<td>R indices (all data)</td>
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<tr>
<td>Type of weighting scheme used</td>
<td>Sigma</td>
</tr>
<tr>
<td>Weighting scheme used</td>
<td>$w = 1/\sigma^2(Fo^2)$</td>
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<tr>
<td>Average shift/error</td>
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<tr>
<td>Largest diff. peak and hole</td>
<td>0.309 and -0.377 eÅ$^3$</td>
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**Special Refinement Details**

Refinement of $F^2$ against ALL reflections. The weighted R-factor ($wR$) and goodness of fit ($S$) are based on $F^2$, conventional R-factors (R) are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(${gt}$) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on $F$, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2\times 10^3$) for SBH05. $U_{eq}$ is defined as the trace of the orthogonalized $U_{ij}$ tensor.

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Table 3. Selected bond lengths [Å] and angles [°] for SBH05.

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**Plane dihedral angle**

Plane 1 – Plane 2 3.48(8)

**Deviations within planes**

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<tr>
<td>C3</td>
<td>0.0018 (0.0017)</td>
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<tr>
<td>C4</td>
<td>0.0256 (0.0017)</td>
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<tr>
<td>C5</td>
<td>0.0077 (0.0017)</td>
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<td>C6</td>
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<td>C15</td>
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<td>-0.0189 (0.0016)</td>
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Table 4. Bond lengths [Å] and angles [°] for SBH05.

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Table 5. Anisotropic displacement parameters ($\AA^2 \times 10^4$) for SBH05. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

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Table 6. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters (Å$^2 \times 10^{-3}$) for SBH05.

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Crystal Structure Analysis of:
(o-NMe₂Ph-QA)Pt(1,2-η²-6-σ-cycloocta-1,4-dienyl) 10a - JCP09

Contents

Table 1. Crystal data
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Table 4. Full bond distances and angles (for deposit)
Table 5. Anisotropic displacement parameters
Table 6. Hydrogen atomic coordinates
Table 7. Observed and calculated structure factors (for deposit)

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 158863. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 158863."
Table 1. Crystal data and structure refinement for JCP09.

Empirical formula  
$C_{25}H_{27}N_5Pt$

Formula weight  
564.59

Crystallization Solvent  
Unknown

Crystal Habit  
Irregular

Crystal size  
$0.22 \times 0.19 \times 0.15 \text{ mm}^3$

Crystal color  
Red

Data Collection

Preliminary Photos  
Rotation

Type of diffractometer  
CCD area detector

Wavelength  
$0.71073 \text{ Å MoK} \alpha$

Data Collection Temperature  
$98(2) \text{ K}$

$\theta$ range for 11348 reflections used in lattice determination  
$2.72$ to $28.28^\circ$

Unit cell dimensions  
$a = 7.5521(7) \text{ Å}$  
$b = 10.7997(9) \text{ Å}$  
$c = 13.4693(12) \text{ Å}$

$1034.23(16) \text{ Å}^3$

Volume  
2

Z  
Triclinic

Crystal system  
P-1

Space group  

Density (calculated)  
$1.813 \text{ Mg/m}^3$

F(000)  
552

Data collection program  
Bruker SMART

$\theta$ range for data collection  
$1.60$ to $28.31^\circ$

Completeness to $\theta = 28.31^\circ$  
$92.4 \%$

Index ranges  
$-9 \leq h \leq 10$, $-14 \leq k \leq 14$, $-17 \leq l \leq 17$

ω scans at $5 \phi$ settings

Data collection scan type  

Data reduction program  
Bruker SAINT v6.2

Reflections collected  
15396

Independent reflections  
4745 [$R_{int} = 0.0365$]

Absorption coefficient  
$6.800 \text{ mm}^{-1}$

Absorption correction  
SADABCS

Max. and min. transmission  
$1.000000$ and $0.728175$
Table 1 (cont.)

Structure solution and Refinement

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Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2σ(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($\AA^2 \times 10^3$) for JCP09. U(eq) is defined as the trace of the orthogonalized Uij tensor.

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Table 3. Selected bond lengths [Å] and angles [°] for JCP09.

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Table 5. Anisotropic displacement parameters (Å² x 10⁶) for JCP09. The anisotropic displacement factor exponent takes the form: -2\pi² [ h² a² U₁₁ + ... + 2 h k a* b* U₁₂ ]

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å² x 10^3) for JCP09.

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Crystal Structure Analysis of:

(3,5-Me₂Ph-QA)Pt(1,2-η²-6-σ-cycloocta-1,4-dienyl) 11- SDB04

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Table 4. Full bond distances and angles (for deposit)
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Table 6. Hydrogen atomic coordinates
Table 7. Observed and calculated structure factors (for deposit)

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 158864. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 158864."
Table 1. Crystal data and structure refinement for SDB04.

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Table 1 (cont.)

Structure solution and Refinement

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Special Refinement Details

The hydrogen atoms of the methyl groups were refined as riding atoms with the torsion angles about the methyl C-C bond free to rotate. All other hydrogen atoms were refined without restraints.

Refinement of F^2 against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2σ(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($\overline{\Delta}^2 x 10^3$) for SDB04. $U_{eq}$ is defined as the trace of the orthogonalized $\overline{\Delta}^2$ tensor.

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