Table S1. Crystal and Intensity Collection Data for 
Pt(bpm)Cl2·0.5(nmp) (3)

Formula: C8Cl2H6N4Pt·0.5(C5H9NO)  
Formula weight: 473.72
Crystal color: Red  
Habit: Short needle
Crystal Size: 0.10 x 0.19 x 0.31 mm  
Crystal System: Monoclinic
Crystal System: Monoclinic  
Space group: C2/m (no. 12)
\(a = 12.668(4) \text{ Å}\)  
\(b = 15.618(6) \text{ Å}\)  
\(c = 6.704(3) \text{ Å}\)
\(V = 1324.0(8) \text{ Å}^3\)  
Lattice parameters: 25 reflections,  
Absorption correction: none
\(\mu = 112.1 \text{ cm}^{-1}\)  
Enraf-Nonius Cad-4 diffractometer  
\(\omega\) scans
MoK\(\alpha\), \(\lambda = 0.7107 \text{ Å}\)  
Graphite monochromator
2\(\theta\) range: 2 - 50°  
\(-15 \leq h \leq 15, -18 \leq k \leq 18, 0 \leq l \leq 7\)
\(T = 294 \text{ K}\)
Number of reflections measured: 2539  
Number of independent reflections: 978
Number with \(F_o^2 > 0\): 900  
Number with \(F_o^2 > 3\sigma(F_o^2)\): 793
Standard reflections: 2 every 150 min.  
Variation: within counting statistics
GOF\(_{\text{merge}}\): 1.30 for 978 multiples  
\(R_{\text{merge}}\): 0.035 for 778 duplicates
Number used in refinement: 978  
Criterion: All reflections used
Final \(R\) on \(F\): 0.031 for 793 reflections with \(F_o^2 > 3\sigma(F_o^2)\)
Final \(R\) on \(F\): 0.038 for 900 reflections with \(F_o^2 > 0\)
Final weighted \(R_w\) on \(F^2\): 0.069
Final GOF: 1.55 for 83 parameters and 978 reflections
\((\Delta/\sigma)_{\text{max}}\) in final least squares cycle: < 0.005
\(\Delta \rho_{\text{max}}\): 1.97 eÅ\(^{-3}\), \(\Delta \rho_{\text{min}}\): -1.46 eÅ\(^{-3}\) in final difference map
Secondary extinction parameter: 0.11(1) x 10\(^{-6}\) (Larson, A. C. Acta Cryst. 1967, 23, 644)

Definitions:
\[R = \frac{\sum|F_o - |F_c||}{\sum F_o}, \quad R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_c^2)^2} \right\}^{1/2}\]
\[GOF = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{n-p} \right\}^{1/2}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}\]
Table S2. Final Heavy Atom Parameters for Pt(bpm)Cl₂·0.5(nmp) (3)

\[ x, y, z \text{ and } U_{eq} \times 10^4 \]

<table>
<thead>
<tr>
<th>Atom</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( U_{eq} ) or ( B )</th>
<th>Multiplicity$^\dagger$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>5203(.4)</td>
<td>0</td>
<td>2508(.8)</td>
<td>267(1)</td>
<td>4.0</td>
</tr>
<tr>
<td>Cl</td>
<td>6488(2)</td>
<td>1035(2)</td>
<td>2487(4)</td>
<td>438(7)</td>
<td>8.0</td>
</tr>
<tr>
<td>N(1)</td>
<td>3991(6)</td>
<td>825(5)</td>
<td>2526(11)</td>
<td>299(19)</td>
<td>8.0</td>
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<tr>
<td>N(2)</td>
<td>2123(6)</td>
<td>897(5)</td>
<td>2397(15)</td>
<td>486(23)</td>
<td>8.0</td>
</tr>
<tr>
<td>C(1)</td>
<td>3028(8)</td>
<td>468(6)</td>
<td>2446(13)</td>
<td>339(23)</td>
<td>8.0</td>
</tr>
<tr>
<td>C(2)</td>
<td>4046(8)</td>
<td>1696(6)</td>
<td>2609(17)</td>
<td>442(27)</td>
<td>8.0</td>
</tr>
<tr>
<td>C(3)</td>
<td>3144(9)</td>
<td>2158(6)</td>
<td>2602(18)</td>
<td>481(28)</td>
<td>8.0</td>
</tr>
<tr>
<td>C(4)</td>
<td>2186(9)</td>
<td>1748(7)</td>
<td>2490(20)</td>
<td>556(31)</td>
<td>8.0</td>
</tr>
<tr>
<td>O</td>
<td>70(17)</td>
<td>1468(9)</td>
<td>5383(25)</td>
<td>0.3(3) *</td>
<td>2.0</td>
</tr>
<tr>
<td>C(5)</td>
<td>-134</td>
<td>751</td>
<td>4610</td>
<td>3.0 *</td>
<td>2.0</td>
</tr>
<tr>
<td>C(6)</td>
<td>-615(20)</td>
<td>487(18)</td>
<td>2814(45)</td>
<td>6.5(7) *</td>
<td>4.0</td>
</tr>
<tr>
<td>C(8)</td>
<td>-34</td>
<td>-721</td>
<td>4697</td>
<td>3.0 *</td>
<td>2.0</td>
</tr>
<tr>
<td>N(3)</td>
<td>215(19)</td>
<td>61(65)</td>
<td>5714(37)</td>
<td>4.1(8) *</td>
<td>2.0</td>
</tr>
<tr>
<td>C(9)</td>
<td>663</td>
<td>151</td>
<td>7743</td>
<td>4.0 *</td>
<td>2.0</td>
</tr>
</tbody>
</table>

$^a \ U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^\tau a_j^\tau)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, \( B \)

$^\dagger$ Number of atoms in the unit cell

Note: Since atom C(7) is related to C(6) by a mirror plane, it was removed from the calculations and C(6) was given double weight.
Table S3. Assigned Hydrogen Atom Parameters for 
Pt(bpm)Cl₂·0.5(nmp) (3)

\( x, y \) and \( z \times 10^4 \)

<table>
<thead>
<tr>
<th>Atom</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>4714</td>
<td>1974</td>
<td>2670</td>
<td>6.0</td>
</tr>
<tr>
<td>H3</td>
<td>3174</td>
<td>2764</td>
<td>2675</td>
<td>7.0</td>
</tr>
<tr>
<td>H4</td>
<td>1556</td>
<td>2076</td>
<td>2481</td>
<td>8.0</td>
</tr>
<tr>
<td>H6A</td>
<td>-212</td>
<td>726</td>
<td>1719</td>
<td>7.0</td>
</tr>
<tr>
<td>H6B</td>
<td>-1309</td>
<td>726</td>
<td>2631</td>
<td>7.0</td>
</tr>
<tr>
<td>H8A</td>
<td>602</td>
<td>-1019</td>
<td>4468</td>
<td>7.0</td>
</tr>
<tr>
<td>H8B</td>
<td>-464</td>
<td>-1065</td>
<td>5489</td>
<td>7.0</td>
</tr>
</tbody>
</table>
Table S4. Anisotropic Displacement Parameters for Pt(bpm)Cl₂·0.5(nmp) (3)

<table>
<thead>
<tr>
<th>Atom</th>
<th>U₁₁</th>
<th>U₂₂</th>
<th>U₃₃</th>
<th>U₁₂</th>
<th>U₁₃</th>
<th>U₂₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>284(4)</td>
<td>211(3)</td>
<td>308(3)</td>
<td>0</td>
<td>37(2)</td>
<td>0</td>
</tr>
<tr>
<td>Cl</td>
<td>382(16)</td>
<td>394(16)</td>
<td>542(17)</td>
<td>-131(12)</td>
<td>52(12)</td>
<td>-25(13)</td>
</tr>
<tr>
<td>N(1)</td>
<td>261(49)</td>
<td>328(46)</td>
<td>310(43)</td>
<td>79(36)</td>
<td>30(32)</td>
<td>31(36)</td>
</tr>
<tr>
<td>N(2)</td>
<td>418(54)</td>
<td>385(47)</td>
<td>659(64)</td>
<td>106(41)</td>
<td>63(45)</td>
<td>-13(47)</td>
</tr>
<tr>
<td>C(1)</td>
<td>426(66)</td>
<td>267(48)</td>
<td>325(55)</td>
<td>-26(46)</td>
<td>25(42)</td>
<td>-37(44)</td>
</tr>
<tr>
<td>C(2)</td>
<td>497(69)</td>
<td>268(49)</td>
<td>564(70)</td>
<td>-51(46)</td>
<td>60(52)</td>
<td>-37(52)</td>
</tr>
<tr>
<td>C(3)</td>
<td>591(75)</td>
<td>269(49)</td>
<td>588(74)</td>
<td>86(55)</td>
<td>70(56)</td>
<td>8(53)</td>
</tr>
<tr>
<td>C(4)</td>
<td>515(75)</td>
<td>419(61)</td>
<td>740(86)</td>
<td>145(56)</td>
<td>78(60)</td>
<td>27(63)</td>
</tr>
</tbody>
</table>

Uᵢ,j values have been multiplied by 10⁴.

The form of the displacement factor is:

\[
\exp \left( \frac{-2\pi^2}{h^2a^*a^* + k^2b^*b^* + l^2c^*c^* + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}k\ell b^*c^*} \right)
\]
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<th>Distance (Å)</th>
<th>Angle (°)</th>
</tr>
</thead>
<tbody>
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<td>2.294(3)</td>
</tr>
<tr>
<td>Pt – N(1)</td>
<td>2.006(8)</td>
</tr>
<tr>
<td>N(1) – C(1)</td>
<td>1.339(12)</td>
</tr>
<tr>
<td>N(1) – C(2)</td>
<td>1.362(13)</td>
</tr>
<tr>
<td>N(2) – C(1)</td>
<td>1.327(13)</td>
</tr>
<tr>
<td>N(2) – C(4)</td>
<td>1.333(15)</td>
</tr>
<tr>
<td>C(1) – C(1)</td>
<td>1.463(13)</td>
</tr>
<tr>
<td>C(2) – C(3)</td>
<td>1.352(15)</td>
</tr>
<tr>
<td>C(3) – C(4)</td>
<td>1.370(16)</td>
</tr>
<tr>
<td>O – C(5)</td>
<td>1.255</td>
</tr>
<tr>
<td>C(6) – C(5)</td>
<td>1.380</td>
</tr>
<tr>
<td>C(6) – C(6)</td>
<td>1.524(4)</td>
</tr>
<tr>
<td>C(6) – C(8)</td>
<td>1.469</td>
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<tr>
<td>N(3) – C(5)</td>
<td>1.365</td>
</tr>
<tr>
<td>N(3) – C(8)</td>
<td>1.425</td>
</tr>
<tr>
<td>N(3) – C(9)</td>
<td>1.449</td>
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<tr>
<td>C(2) – H2</td>
<td>0.949</td>
</tr>
<tr>
<td>C(3) – H3</td>
<td>0.949</td>
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<tr>
<td>C(4) – H4</td>
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</tr>
<tr>
<td>C(6) – H6A</td>
<td>0.947</td>
</tr>
<tr>
<td>C(6) – H6B</td>
<td>0.957</td>
</tr>
<tr>
<td>C(8) – H8A</td>
<td>0.950</td>
</tr>
<tr>
<td>C(8) – H8B</td>
<td>0.950</td>
</tr>
<tr>
<td>N(1) – Pt</td>
<td>2.519</td>
</tr>
<tr>
<td>Pt – N(1)</td>
<td>2.006(8)</td>
</tr>
<tr>
<td>Pt – C(1)</td>
<td>1.339(12)</td>
</tr>
<tr>
<td>N(1) – C(2)</td>
<td>1.362(13)</td>
</tr>
<tr>
<td>N(2) – C(1)</td>
<td>1.327(13)</td>
</tr>
<tr>
<td>N(2) – C(4)</td>
<td>1.333(15)</td>
</tr>
<tr>
<td>C(1) – C(1)</td>
<td>1.463(13)</td>
</tr>
<tr>
<td>C(2) – C(3)</td>
<td>1.352(15)</td>
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<tr>
<td>C(3) – C(4)</td>
<td>1.370(16)</td>
</tr>
<tr>
<td>C(4) – N(2)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
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<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
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<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
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<td>C(4) – N(1)</td>
<td>1.167(6)</td>
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<td>C(4) – N(1)</td>
<td>1.167(6)</td>
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<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
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<td>C(4) – N(1)</td>
<td>1.167(6)</td>
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<td>1.175(8)</td>
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<td>1.167(6)</td>
</tr>
<tr>
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<td>1.175(8)</td>
</tr>
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<td>1.167(6)</td>
</tr>
<tr>
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<td>1.175(8)</td>
</tr>
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<td>1.167(6)</td>
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<tr>
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<td>1.175(8)</td>
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<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.175(8)</td>
</tr>
<tr>
<td>C(4) – N(1)</td>
<td>1.167(6)</td>
</tr>
</tbody>
</table>
Table S6. Crystal and Intensity Collection Data for Pt(phen)(CN)₂ (6)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula: C₁₄H₈N₄Pt</td>
<td>Formula weight: 427.32</td>
</tr>
<tr>
<td>Crystal color: Violet</td>
<td>Habit: Thin needle</td>
</tr>
<tr>
<td>Crystal Size: 0.02 x 0.06 x 0.20 mm</td>
<td>ρ.calc = 2.38 g cm⁻³</td>
</tr>
<tr>
<td>Crystal System: Orthorhombic</td>
<td>Space group: Pbcα (no. 61)</td>
</tr>
<tr>
<td>a = 38.731(13) Å</td>
<td></td>
</tr>
<tr>
<td>b = 18.569(3) Å</td>
<td></td>
</tr>
<tr>
<td>c = 6.628(1) Å</td>
<td></td>
</tr>
<tr>
<td>V = 4766(2) Å³</td>
<td>Z = 16</td>
</tr>
<tr>
<td>Lattice parameters: 25 reflections,</td>
<td>8.3° ≤ θ ≤ 10.1°</td>
</tr>
<tr>
<td>μ = 118.9 cm⁻¹</td>
<td>Relative transmission: 0.83 – 1.09</td>
</tr>
<tr>
<td>Enraf-Nonius Cad-4 diffractometer</td>
<td>ω scans</td>
</tr>
<tr>
<td>MoKα, λ = 0.7107 Å</td>
<td>Graphite monochromator</td>
</tr>
<tr>
<td>2θ range: 2 – 40°</td>
<td></td>
</tr>
<tr>
<td>T = 294 K</td>
<td></td>
</tr>
<tr>
<td>Number of reflections measured: 10428</td>
<td>Number of independent reflections: 2213</td>
</tr>
<tr>
<td>Number with F₀² &gt; 0: 1754</td>
<td>Number with F₀² &gt; 3σ(F₀²): 1221</td>
</tr>
<tr>
<td>Standard reflections: 3 every 90 min.</td>
<td>Variation: within counting statistics</td>
</tr>
<tr>
<td>GOF_merge: 0.98 for 2213 multiples</td>
<td>R_merge: 0.0326 for 78 duplicates</td>
</tr>
<tr>
<td>Number used in refinement: 2213</td>
<td>Criterion: All reflections used</td>
</tr>
<tr>
<td>Final R on F: 0.041 for 1221 reflections with F₀² &gt; 3σ(F₀²)</td>
<td></td>
</tr>
<tr>
<td>Final R on F: 0.069 for 1754 reflections with F₀² &gt; 0</td>
<td></td>
</tr>
<tr>
<td>Final weighted R_w on F²: 0.086</td>
<td></td>
</tr>
<tr>
<td>Final GOF: 1.61 for 164 parameters and 2213 reflections</td>
<td>(Δ/σ)max in final least squares cycle: 0.01</td>
</tr>
<tr>
<td>Δρ_max: 3.46 eÅ⁻³, Δρ_min: -2.65 eÅ⁻³ in final difference map</td>
<td></td>
</tr>
<tr>
<td>Secondary extinction parameter: 0.0039(11) x 10⁻⁶ (Larson, A. C. Acta Cryst. 1967, 22, 644)</td>
<td></td>
</tr>
</tbody>
</table>

Definitions:

\[ R = \frac{\sum|F_o|-|F_c|}{\sum F_o} \]

\[ R_w = \left\{ \frac{\sum w(F_o^2-F_c^2)}{\sum w(F_o^2)^2} \right\}^{\frac{1}{2}} \]

\[ GOF = \left\{ \frac{\sum w(F_o^2-F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}, \text{ where } n = \text{number of data}, p = \text{number of parameters refined.} \]
Table S7. Final Heavy Atom Parameters for

Pt(phen)(CN)$_2$ (6)

$x, y, z$ and $U_{eq} \times 10^4$

<table>
<thead>
<tr>
<th>Atom</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$U_{eq}$ or $B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt1</td>
<td>379.3</td>
<td>2407(1)</td>
<td>3109(1)</td>
<td>295(3)</td>
</tr>
<tr>
<td>Pt2</td>
<td>2878.3</td>
<td>2393(1)</td>
<td>2970(1)</td>
<td>264(2)</td>
</tr>
<tr>
<td>N1</td>
<td>221(7 )</td>
<td>3476(12)</td>
<td>2929(30)</td>
<td>2.9(5)*</td>
</tr>
<tr>
<td>N2</td>
<td>853(5 )</td>
<td>2897(9 )</td>
<td>3396(31)</td>
<td>2.7(4)*</td>
</tr>
<tr>
<td>N3</td>
<td>-369(14)</td>
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\[ U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)] \]

* Isotropic displacement parameter, $B$
Table S8. Assigned Hydrogen Atom Parameters for Pt(phen)(CN)$_2$ (6)

$x, y$ and $z \times 10^4$

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Table S9. Platinum Atom Anisotropic Displacement Parameters for Pt(phen)(CN)₂ (6)

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$U_{ij}$ values have been multiplied by $10^4$

The form of the displacement factor is:

$$\exp \left(-2\pi^2 \left( U_{11} h^2 a^* a^* + U_{22} k^2 b^* b^* + U_{33} l^2 c^* c^* + 2 U_{12} h k a^* b^* + 2 U_{13} h l a^* c^* + 2 U_{23} k l b^* c^* \right) \right)$$
Table S10. Complete Distances and Angles for Pt(phen)(CN)$_2$ (6)

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</table>
Table S11. Crystal and Intensity Collection Data for Pt(bpy)(NCS)$_2$ (7)

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula: C$_{12}$H$_8$N$_4$PtS$_2$</td>
<td>Formula weight: 467.43</td>
</tr>
<tr>
<td>Crystal color: Red</td>
<td>Habit: Blade</td>
</tr>
<tr>
<td>Crystal Size: 0.03 x 0.06 x 0.41 mm</td>
<td>$\rho_{\text{calc}} = 2.29 \text{ g cm}^{-3}$</td>
</tr>
<tr>
<td>Crystal System: Orthorhombic</td>
<td>Space group: Pbcm (no. 57)</td>
</tr>
<tr>
<td>$a = 10.349(3)$ Å</td>
<td></td>
</tr>
<tr>
<td>$b = 19.927(5)$ Å</td>
<td></td>
</tr>
<tr>
<td>$c = 6.572(3)$ Å</td>
<td></td>
</tr>
<tr>
<td>$V = 1355.3(7)$ Å$^3$</td>
<td>$Z = 4$</td>
</tr>
<tr>
<td>Lattice parameters: 25 reflections,</td>
<td>$9^\circ \leq \theta \leq 11^\circ$</td>
</tr>
<tr>
<td>$\mu = 107.4$ cm$^{-1}$</td>
<td>Absorption correction: none</td>
</tr>
<tr>
<td>Enraf-Nonius Cad-4 diffractometer</td>
<td>$\omega$ scans</td>
</tr>
<tr>
<td>MoK$_\alpha$, $\lambda = 0.7107$ Å</td>
<td>Graphite monochromator</td>
</tr>
<tr>
<td>$2\theta$ range: 2$^\circ$ - 40$^\circ$</td>
<td>$0 \leq h \leq 9, 0 \leq k \leq 19, -6 \leq l \leq 6$</td>
</tr>
<tr>
<td>$T = 294$ K</td>
<td></td>
</tr>
<tr>
<td>Number of reflections measured: 1626</td>
<td>Number of independent reflections: 710</td>
</tr>
<tr>
<td>Number with $F_0^2 &gt; 0$: 643</td>
<td>Number with $F_0^2 &gt; 3\sigma(F_0^2)$: 565</td>
</tr>
<tr>
<td>Standard reflections: 3 every 150 min.</td>
<td>Variation: within counting statistics</td>
</tr>
<tr>
<td>GOF$_{\text{merge}}$: 1.06 for 709 multiples</td>
<td>$R_{\text{merge}}$: 0.019 for 629 duplicates</td>
</tr>
<tr>
<td>Number used in refinement: 710</td>
<td>Criterion: All reflections used</td>
</tr>
<tr>
<td>Final R on F: 0.044 for 565 reflections with $F_0^2 &gt; 3\sigma(F_0^2)$</td>
<td></td>
</tr>
<tr>
<td>Final R on F: 0.050 for 643 reflections with $F_0^2 &gt; 0$</td>
<td></td>
</tr>
<tr>
<td>Final weighted $R_w$ on $F^2$: 0.099</td>
<td></td>
</tr>
<tr>
<td>Final GOF: 2.80 for 67 parameters and 710 reflections</td>
<td></td>
</tr>
<tr>
<td>$(\Delta/\sigma)_{\text{max}}$ in final least squares cycle: &lt; 0.01</td>
<td></td>
</tr>
<tr>
<td>$\Delta\rho_{\text{max}}$: 1.68 eÅ$^{-3}$, $\Delta\rho_{\text{min}}$: -1.49 eÅ$^{-3}$ in final difference map</td>
<td></td>
</tr>
</tbody>
</table>

Definitions:

$$R = \frac{\Sigma|F_2 - |F_z||}{\Sigma F_z}; \quad R_w = \left\{ \frac{\Sigma w(F_2^2 - F_z^2)^2}{\Sigma w(F_z^2)^2} \right\}^{\frac{1}{2}}$$

$$\text{GOF} = \left\{ \frac{\Sigma w(F_2^2 - F_z^2)^2}{n - p} \right\}^{\frac{1}{2}}$$

where $n =$ number of data, $p =$ number of parameters refined.
Table S12. Final Heavy Atom Parameters for 

\( \text{Pt(bpy)(NCS)\textsubscript{2}} \) (7)

\( x, y, z \) and \( U_{eq} \times 10^4 \)

<table>
<thead>
<tr>
<th>Atom</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( U_{eq} ) or ( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>1495(1)</td>
<td>2572(1)</td>
<td>2500</td>
<td>562(3)</td>
</tr>
<tr>
<td>N1</td>
<td>-219(22)</td>
<td>2964(10)</td>
<td>2500</td>
<td>4.9(5) *</td>
</tr>
<tr>
<td>C1</td>
<td>-1145(26)</td>
<td>3241(12)</td>
<td>2500</td>
<td>5.1(6) *</td>
</tr>
<tr>
<td>S1</td>
<td>-2572(10)</td>
<td>3645(4)</td>
<td>2500</td>
<td>1076(30)</td>
</tr>
<tr>
<td>N2</td>
<td>2286(26)</td>
<td>3546(12)</td>
<td>2500</td>
<td>6.2(6) *</td>
</tr>
<tr>
<td>C2</td>
<td>2850(30)</td>
<td>3982(14)</td>
<td>2500</td>
<td>5.7(7) *</td>
</tr>
<tr>
<td>S2</td>
<td>3615(10)</td>
<td>4659(4)</td>
<td>2500</td>
<td>1179(32)</td>
</tr>
<tr>
<td>N3</td>
<td>806(22)</td>
<td>1603(10)</td>
<td>2500</td>
<td>5.2(5) *</td>
</tr>
<tr>
<td>C3</td>
<td>-331(28)</td>
<td>1379(12)</td>
<td>2500</td>
<td>5.0(6) *</td>
</tr>
<tr>
<td>C4</td>
<td>-610(30)</td>
<td>725(13)</td>
<td>2500</td>
<td>5.9(7) *</td>
</tr>
<tr>
<td>C5</td>
<td>279(28)</td>
<td>290(12)</td>
<td>2500</td>
<td>5.4(6) *</td>
</tr>
<tr>
<td>C6</td>
<td>1576(28)</td>
<td>474(12)</td>
<td>2500</td>
<td>5.8(6) *</td>
</tr>
<tr>
<td>C7</td>
<td>1927(23)</td>
<td>1139(11)</td>
<td>2500</td>
<td>4.0(6) *</td>
</tr>
<tr>
<td>C8</td>
<td>3166(25)</td>
<td>1460(11)</td>
<td>2500</td>
<td>4.1(6) *</td>
</tr>
<tr>
<td>C9</td>
<td>4249(29)</td>
<td>1069(12)</td>
<td>2500</td>
<td>5.3(6) *</td>
</tr>
<tr>
<td>C10</td>
<td>5414(33)</td>
<td>1410(14)</td>
<td>2500</td>
<td>6.6(7) *</td>
</tr>
<tr>
<td>C11</td>
<td>5477(30)</td>
<td>2058(14)</td>
<td>2500</td>
<td>6.5(7) *</td>
</tr>
<tr>
<td>C12</td>
<td>4326(24)</td>
<td>2409(12)</td>
<td>2500</td>
<td>4.9(5) *</td>
</tr>
<tr>
<td>N4</td>
<td>3139(17)</td>
<td>2134(9)</td>
<td>2500</td>
<td>3.6(4) *</td>
</tr>
</tbody>
</table>

\( ^* \) \( U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)] \)

* Isotropic displacement parameter, \( B \)
Table S13. Assigned Hydrogen Atom Parameters for Pt(bpy)(NCS)$_2$ (7)

\[ z, y \text{ and } z \times 10^4 \]

<table>
<thead>
<tr>
<th>Atom</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>H3</td>
<td>-1057</td>
<td>1704</td>
<td>2500</td>
<td>6.1</td>
</tr>
<tr>
<td>H4</td>
<td>-1521</td>
<td>581</td>
<td>2500</td>
<td>6.7</td>
</tr>
<tr>
<td>H5</td>
<td>46</td>
<td>-182</td>
<td>2500</td>
<td>6.5</td>
</tr>
<tr>
<td>H6</td>
<td>2231</td>
<td>127</td>
<td>2500</td>
<td>6.4</td>
</tr>
<tr>
<td>H9</td>
<td>4253</td>
<td>577</td>
<td>2500</td>
<td>6.5</td>
</tr>
<tr>
<td>H10</td>
<td>6203</td>
<td>1150</td>
<td>2500</td>
<td>7.3</td>
</tr>
<tr>
<td>H11</td>
<td>6307</td>
<td>2283</td>
<td>2500</td>
<td>7.5</td>
</tr>
<tr>
<td>H12</td>
<td>4404</td>
<td>2895</td>
<td>2500</td>
<td>5.7</td>
</tr>
</tbody>
</table>
Table S14. Anisotropic Displacement Parameters for Pt(bpy)(NCS)$_2$ (7)

<table>
<thead>
<tr>
<th>Atom</th>
<th>$U_{11}$</th>
<th>$U_{22}$</th>
<th>$U_{33}$</th>
<th>$U_{12}$</th>
<th>$U_{13}$</th>
<th>$U_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>753(8)</td>
<td>498(7)</td>
<td>436(7)</td>
<td>24(8)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>S1</td>
<td>940(71)</td>
<td>793(54)</td>
<td>1496(96)</td>
<td>67(52)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>S2</td>
<td>1254(83)</td>
<td>737(50)</td>
<td>1546(97)</td>
<td>-72(60)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

$U_{ij}$ values have been multiplied by $10^4$

The form of the displacement factor is:

$$
\exp -2\pi^2(U_{11}h^2a^* + U_{22}k^2b^* + U_{33}\ell^2c^* + 2U_{12}hka^*b^* + 2U_{13}hka^*c^* + 2U_{23}k\ell b^*c^*)
$$
Table S15. Complete Distances and Angles for Pt(bpy)(NCS)$_2$ (7)

<table>
<thead>
<tr>
<th>Distance (Å)</th>
<th>Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt – N1</td>
<td>1.94(2)</td>
</tr>
<tr>
<td>Pt – N2</td>
<td>2.11(3)</td>
</tr>
<tr>
<td>Pt – N3</td>
<td>2.06(2)</td>
</tr>
<tr>
<td>Pt – N4</td>
<td>1.912(17)</td>
</tr>
<tr>
<td>N1 – C1</td>
<td>1.11(3)</td>
</tr>
<tr>
<td>C1 – S1</td>
<td>1.68(3)</td>
</tr>
<tr>
<td>N2 – C2</td>
<td>1.05(4)</td>
</tr>
<tr>
<td>C2 – S2</td>
<td>1.57(3)</td>
</tr>
<tr>
<td>N3 – C3</td>
<td>1.26(3)</td>
</tr>
<tr>
<td>N3 – C7</td>
<td>1.48(3)</td>
</tr>
<tr>
<td>C3 – C4</td>
<td>1.34(4)</td>
</tr>
<tr>
<td>C4 – C5</td>
<td>1.26(4)</td>
</tr>
<tr>
<td>C5 – C6</td>
<td>1.39(4)</td>
</tr>
<tr>
<td>C6 – C7</td>
<td>1.37(4)</td>
</tr>
<tr>
<td>C7 – C8</td>
<td>1.43(3)</td>
</tr>
<tr>
<td>C8 – C9</td>
<td>1.36(4)</td>
</tr>
<tr>
<td>C8 – N4</td>
<td>1.34(3)</td>
</tr>
<tr>
<td>C8 – C9</td>
<td>1.36(4)</td>
</tr>
<tr>
<td>C9 – C10</td>
<td>1.38(4)</td>
</tr>
<tr>
<td>C10 – C11</td>
<td>1.29(4)</td>
</tr>
<tr>
<td>C11 – C12</td>
<td>1.38(4)</td>
</tr>
<tr>
<td>C12 – N4</td>
<td>1.35(3)</td>
</tr>
<tr>
<td>C3 – H3</td>
<td>0.991</td>
</tr>
<tr>
<td>C4 – H4</td>
<td>0.985</td>
</tr>
<tr>
<td>C5 – H5</td>
<td>0.970</td>
</tr>
<tr>
<td>C6 – H6</td>
<td>0.969</td>
</tr>
<tr>
<td>C9 – H9</td>
<td>0.982</td>
</tr>
<tr>
<td>C10 – H10</td>
<td>0.968</td>
</tr>
<tr>
<td>C11 – H11</td>
<td>0.970</td>
</tr>
<tr>
<td>C12 – H12</td>
<td>0.973</td>
</tr>
<tr>
<td>H3 – C3 – N3</td>
<td>118.4</td>
</tr>
<tr>
<td>H3 – C3 – C4</td>
<td>118.2</td>
</tr>
<tr>
<td>H4 – C4 – C3</td>
<td>119.4</td>
</tr>
<tr>
<td>H4 – C4 – C5</td>
<td>119.8</td>
</tr>
<tr>
<td>H5 – C5 – C4</td>
<td>118.9</td>
</tr>
</tbody>
</table>
Table 15. (Cont.)

<table>
<thead>
<tr>
<th>Angle(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H5 -C5 -C6</td>
</tr>
<tr>
<td>H6 -C6 -C5</td>
</tr>
<tr>
<td>H6 -C6 -C7</td>
</tr>
<tr>
<td>H9 -C9 -C8</td>
</tr>
<tr>
<td>H9 -C9 -C10</td>
</tr>
<tr>
<td>H10 -C10 -C9</td>
</tr>
<tr>
<td>H10 -C10 -C11</td>
</tr>
<tr>
<td>H11 -C11 -C10</td>
</tr>
<tr>
<td>H11 -C11 -C12</td>
</tr>
<tr>
<td>H12 -C12 -C11</td>
</tr>
<tr>
<td>H12 -C12 -N4</td>
</tr>
</tbody>
</table>
Table S16. Crystal and Intensity Collection Data for 
Pt(dmbpy)(NCO)$_2$ (1b)

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula: $C_{14}H_{12}N_4O_2Pt$</td>
<td>Formula weight: 463.36</td>
</tr>
<tr>
<td>Crystal color: Yellow</td>
<td>Habit: Rectangular prisms</td>
</tr>
<tr>
<td>Crystal Size: 0.11 x 0.14 x 0.22 mm</td>
<td>( \rho_{\text{calc}} = 2.22 \text{ g cm}^{-3} )</td>
</tr>
<tr>
<td>Crystal System: Monoclinic</td>
<td>Space group: $C2/c$ (no. 15)</td>
</tr>
<tr>
<td>( a = 17.313(4) \text{ Å} )</td>
<td>( \beta = 114.00(2)^\circ )</td>
</tr>
<tr>
<td>( b = 12.263(3) \text{ Å} )</td>
<td>( Z = 8 )</td>
</tr>
<tr>
<td>( c = 14.291(4) \text{ Å} )</td>
<td>Lattice parameters: 25 reflections, ( 4.5^\circ \leq \theta \leq 14.5^\circ )</td>
</tr>
<tr>
<td>( V = 2771.8(11) \text{ Å}^3 )</td>
<td>Relative transmission: 0.85 – 1.16</td>
</tr>
<tr>
<td>Enraf-Nonius Cad-4 diffractometer</td>
<td>( \theta - 2\theta ) scans</td>
</tr>
<tr>
<td>MoK( \alpha ), ( \lambda = 0.7107 \text{ Å} )</td>
<td>Graphite monochromator</td>
</tr>
<tr>
<td>2( \theta ) range: 2 – 50( ^\circ )</td>
<td></td>
</tr>
<tr>
<td>( T = 294 \text{ K} )</td>
<td>Number of reflections measured: 4737</td>
</tr>
<tr>
<td>Number of independent reflections: 2016</td>
<td>Number with ( F_o^2 &gt; 0 ): 1920</td>
</tr>
<tr>
<td>Number with ( F_o^2 &gt; 3\sigma(F_o^2) ): 1605</td>
<td>Number with ( F_o^2 &gt; 3\sigma(F_o^2) ): 1605</td>
</tr>
<tr>
<td>Standard reflections: 3 every 150 min.</td>
<td>Variation: within counting statistics</td>
</tr>
<tr>
<td>GOF$_{\text{merge}}$: 1.07 for 1925 multiples</td>
<td>R$_{\text{merge}}$: 0.026 for 1652 duplicates</td>
</tr>
<tr>
<td>Number used in refinement: 2016</td>
<td>Criterion: All reflections used</td>
</tr>
<tr>
<td>Final R on F: 0.022 for 1605 reflections with ( F_o^2 &gt; 3\sigma(F_o^2) )</td>
<td></td>
</tr>
<tr>
<td>Final R on F: 0.031 for 1920 reflections with ( F_o^2 &gt; 0 )</td>
<td></td>
</tr>
<tr>
<td>Final weighted R$_w$ on F$^2$: 0.048</td>
<td></td>
</tr>
<tr>
<td>Final GOF: 1.24 for 191 parameters and 2016 reflections</td>
<td></td>
</tr>
<tr>
<td>( (\Delta/\sigma)_{\text{max}} ) in final least squares cycle: &lt; 0.005</td>
<td></td>
</tr>
<tr>
<td>( \Delta \rho_{\text{max}} ): 0.76 eÅ$^{-3}$, ( \Delta \rho_{\min} ): -0.72 eÅ$^{-3}$ in final difference map</td>
<td></td>
</tr>
<tr>
<td>Secondary extinction parameter: 0.083(4) x 10$^{-6}$ (Larson, A. C. Acta Cryst. 1967, 23, 644)</td>
<td></td>
</tr>
</tbody>
</table>

Definitions:

\[
R = \frac{\sum |F_o| - |F_x|}{\sum |F_o|}, \quad R_w = \left( \frac{\sum w(F_o^2-F_x^2)^2}{\sum w(F_o^2)^2} \right)^{\frac{1}{2}}
\]

\[
GOF = \left( \frac{\sum w(F_o^2-F_x^2)^2}{n-p} \right)^{\frac{1}{2}}, \text{ where } n = \text{number of data, } p = \text{number of parameters refined.}
\]
Table S17. Final Heavy Atom Parameters for

$\text{Pt(dmbpy)(NCO)}_2$ (1b)

$x, y, z$ and $U_{eq}^a \times 10^4$

<table>
<thead>
<tr>
<th>Atom</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$U_{eq}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>1361(1)</td>
<td>93(.2)</td>
<td>1527(.2)</td>
<td>366(1)</td>
</tr>
<tr>
<td>N1</td>
<td>1841(3)</td>
<td>-1375(4)</td>
<td>1520(4)</td>
<td>542(15)</td>
</tr>
<tr>
<td>C1</td>
<td>2147(4)</td>
<td>-2086(6)</td>
<td>1283(5)</td>
<td>506(19)</td>
</tr>
<tr>
<td>O1</td>
<td>2458(3)</td>
<td>-2867(4)</td>
<td>1061(4)</td>
<td>827(16)</td>
</tr>
<tr>
<td>N2</td>
<td>2490(3)</td>
<td>766(4)</td>
<td>1806(5)</td>
<td>579(16)</td>
</tr>
<tr>
<td>C2</td>
<td>3183(5)</td>
<td>939(5)</td>
<td>2296(6)</td>
<td>563(20)</td>
</tr>
<tr>
<td>O2</td>
<td>3909(3)</td>
<td>1160(4)</td>
<td>2780(5)</td>
<td>977(21)</td>
</tr>
<tr>
<td>N3</td>
<td>204(3)</td>
<td>-464(4)</td>
<td>1274(3)</td>
<td>359(12)</td>
</tr>
<tr>
<td>C3</td>
<td>-28(4)</td>
<td>-1504(5)</td>
<td>1237(5)</td>
<td>437(17)</td>
</tr>
<tr>
<td>C4</td>
<td>-839(4)</td>
<td>-1806(5)</td>
<td>1090(5)</td>
<td>463(17)</td>
</tr>
<tr>
<td>C5</td>
<td>-1436(3)</td>
<td>-1013(5)</td>
<td>973(4)</td>
<td>405(16)</td>
</tr>
<tr>
<td>C6</td>
<td>-2330(4)</td>
<td>-1278(5)</td>
<td>798(6)</td>
<td>570(18)</td>
</tr>
<tr>
<td>C7</td>
<td>-1195(3)</td>
<td>65(5)</td>
<td>1005(4)</td>
<td>403(15)</td>
</tr>
<tr>
<td>C8</td>
<td>-387(3)</td>
<td>332(4)</td>
<td>1158(4)</td>
<td>326(13)</td>
</tr>
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Table 17. (Cont.)

<table>
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<tr>
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<th>z</th>
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\[ U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\mathbf{a}_i \cdot \mathbf{a}_j)] \]
Table S18. Assigned Hydrogen Atom Parameters for Pt(dmbpy)(NCO)$_2$ (1b)

$x, y$ and $z \times 10^4$

<table>
<thead>
<tr>
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<th>$z$</th>
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<td>185</td>
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<td>1359</td>
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Table S19. Anisotropic Displacement Parameters for Pt(dmbpy)(NCO)$_2$ (1b)

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<th>$U_{22}$</th>
<th>$U_{33}$</th>
<th>$U_{12}$</th>
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<td>353(2)</td>
<td>37(1)</td>
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<td>616(40)</td>
<td>222(27)</td>
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<td>22(29)</td>
</tr>
<tr>
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<td>433(43)</td>
<td>10(34)</td>
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<td>91(34)</td>
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<td>670(42)</td>
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<td>249(31)</td>
<td>23(31)</td>
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<td>422(39)</td>
<td>796(57)</td>
<td>6(32)</td>
<td>278(42)</td>
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<td>399(32)</td>
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$U_{i,j}$ values have been multiplied by $10^4$

The form of the displacement factor is:

$$
\exp(-2\pi^2(U_{11}h^2a^*a^* + U_{22}k^2b^*b^* + U_{33}\ell^2c^*c^* + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}k\ell b^*c^*)
$$
Table S20. Complete Distances and Angles for Pt(dmbpy)(NCO)$_2$ (1b)

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<th>Distance(Å)</th>
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<td>Pt -N2</td>
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<tr>
<td>Pt -N3</td>
<td>2.005(5)</td>
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<tr>
<td>Pt -N4</td>
<td>2.001(5)</td>
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<tr>
<td>N1 -C1</td>
<td>1.141(9)</td>
</tr>
<tr>
<td>C1 -O1</td>
<td>1.203(9)</td>
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<td>1.136(9)</td>
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<tr>
<td>C2 -O2</td>
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<td>1.332(8)</td>
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<td>N3 -C8</td>
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<tr>
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Table 20. (Cont.)

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<td>H4 -C4 -C3 120.3</td>
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</tr>
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