

**Electronic Supplementary Material for:**

**An efficient Stereospecific Synthesis of Polysubstituted *E*-Olefins by Reaction of Acyclic Nitrones with Free and Platinum(II) Coordinated Organonitriles**

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## Material and instrumentation

Methylene chloride ( $\text{CH}_2\text{Cl}_2$ ) was distilled from calcium hydride. C, H and N elemental analyses were carried out by the Microanalytical Service of the Instituto Superior Técnico.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{195}\text{Pt}$  NMR spectra (in  $\text{CDCl}_3$ ) were measured on a Varian Unity 300 spectrometer at ambient temperature. Positive-ion FAB mass spectra were obtained on a Trio 2000 instrument by bombarding 3-nitrobenzyl alcohol (NBA) matrixes of samples with 8 keV (*ca*  $1.28 \times 10^{15}$  J) Xe atoms.  $^1\text{H}$ ,  $^{13}\text{C}$  chemical shifts ( $\delta$ ) were expressed in ppm relative to  $\text{Si}(\text{Me})_4$  and  $^{195}\text{Pt}$  chemical shifts are relative to  $\text{Na}_2[\text{PtCl}_6]$  (by using aqueous  $\text{K}_2[\text{PtCl}_4]$ ,  $\delta = -1630$  ppm, as a standart) with half-height line width in parentheses.  $J$  values are in Hertz. Infrared spectra ( $4000\text{-}400\text{ cm}^{-1}$ ) were recorded on a Bio-Rad FTS 3000MX and a Jasco FT/IR-430 instruments in KBr pellets and the wavenumbers are in  $\text{cm}^{-1}$ . The microwave irradiation experiments were undertaken in a focused microwave CEM Discover reactor (10 mL, 13 mm diameter, 300 W) which is fitted with a rotational system and an IR detector of temperature.

## Crystal structure determinations of 3a and 5c

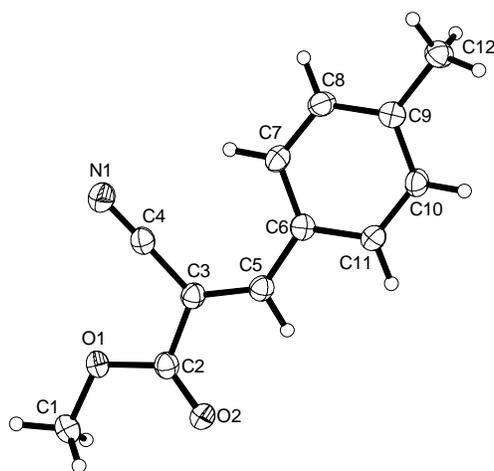
The X-ray diffraction data were collected with a Nonius KappaCCD diffractometer using Mo  $\text{K}\alpha$  radiation ( $\lambda = 0.71073\text{ \AA}$ ). The single crystals were mounted in inert oil within the cold gas stream of the diffractometer. The Denzo-Scalepack<sup>1</sup> or EvalCCD<sup>2</sup> program packages were used for cell refinements and data reduction. Structures were solved by direct methods using the SHELXS<sup>3</sup> or SIR2004<sup>4</sup> programs. A multiscan absorption correction based on equivalent reflections (SADABS)<sup>5</sup> was applied to **5c** ( $T_{\text{min}}/T_{\text{max}}$  0.4030/0.7937). The structures were refined against  $F^2$  using SHELXL-97<sup>6</sup> and WinGX<sup>7</sup> graphical user interface. All hydrogens were placed

in idealized position and constrained to ride on their parent atom. The crystallographic data are summarized in Table 1 and selected bond lengths and angles in Figure captions (Figures 1 and 2).

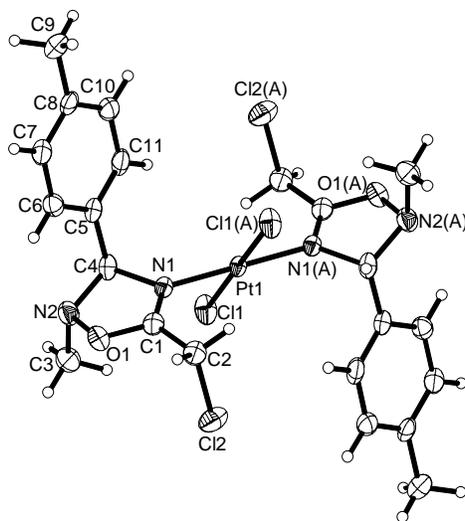
**Table 1:** Crystallographic data for the alkene (NC)(CO<sub>2</sub>Me)C=C(H)(4-MeC<sub>6</sub>H<sub>4</sub>) **3a** and the complex [PtCl<sub>2</sub>{N=C(CH<sub>2</sub>Cl)ON(Me)C(H)(4-MeC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>}] **5c**.

	<b>3a</b>	<b>5c</b>
empirical formula	C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>22</sub> H <sub>26</sub> Cl <sub>4</sub> N <sub>4</sub> O <sub>2</sub> Pt
Fw	201.22	715.36
Temp (K)	100(2) K	120(2)
$\lambda$ (Å)	0.71073	0.71073
cryst syst	Triclinic	Monoclinic
space group	P $\bar{1}$	P2 <sub>1</sub> /c
$a$ (Å)	3.9990(4)	9.3767(6)
$b$ (Å)	11.1539(11)	20.656(3)
$c$ (Å)	12.2250(10)	6.6342(5)
$\alpha$ (deg)	71.924(5)	90
$\beta$ (deg)	89.510(8)	92.122(5)
$\gamma$	81.010(5)	90
$V$ (Å <sup>3</sup> )	511.55(8)	1284.0(2)
$Z$	2	2
$\rho_{\text{calc}}$ (Mg/m <sup>3</sup> )	1.306	1.850
$\mu$ (Mo K $\alpha$ ) (mm <sup>-1</sup> )	0.090	5.907
no. of collected rflns	2965	15313
no. of unique rflns	1765	2916
$R_{\text{int}}$	0.0272	0.0493
$R1^a$ ( $I \geq 2\sigma$ )	0.0491	0.0275
$wR2^b$ ( $I \geq 2\sigma$ )	0.1200	0.0477

$$^a RI = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}.$$



**Figure 1:** Molecular structure of the alkene (NC)(CO<sub>2</sub>Me)C=C(H)(4-MeC<sub>6</sub>H<sub>4</sub>) **3a** with atomic numbering scheme. Selected bond lengths [Å] and angles [°]: C(1)-O(1), 1.449(2); C(2)-O(2), 1.206(2); C(2)-O(1), 1.343(2); C(2)-C(3), 1.488(3); C(3)-C(5), 1.349(3), C(3)-C(4), 1.435(3); N(1)-C(4), 1.149(3); C(5)-C(6), 1.457(3); O(2)-C(2)-O(1), 124.0(2); O(2)-C(2)-C(3), 124.4(2); C(5)-C(3)-C(4), 125.0(2); N(1)-C(4)-C(3), 178.6(2); C(2)-O(1)-C(1), 115.60(15).



**Figure 2:** Molecular structure of the complex *trans*-[PtCl<sub>2</sub>{N=C(CH<sub>2</sub>Cl)ON(Me)C(H)(4-MeC<sub>6</sub>H<sub>4</sub>)}<sub>2</sub>] **5c** with atomic numbering scheme. Selected bond lengths [Å] and angles [°]: Pt(1)-N(1), 2.004(3); Pt(1)-Cl(1), 2.2849(9); Cl(2)-C(2), 1.786(4); O(1)-C(1), 1.349(5); O(1)-N(2), 1.496(4); N(1)-C(4), 1.489(5); N(2)-C(3), 1.473(5); N(2)-C(4), 1.477(5); C(1)-C(2), 1.483(6); C(4)-C(5), 1.509(5); N(1)-Pt(1)-Cl(1), 87.10(8); C(1)-O(1)-N(2), 105.4(3); C(1)-N(1)-C(4), 107.1(3); C(3)-N(2)-C(4), 111.8(3); C(3)-N(2)-O(1), 104.0(3); C(4)-N(2)-O(1), 101.6(3); N(1)-C(1)-O(1), 115.5(3); C(1)-C(2)-Cl(2), 108.2(3); N(2)-C(4)-N(1), 103.4(3).

**Tables 2-6** Crystallographic data, atomic coordinates, bond lengths, bond angles, anisotropic displacement parameters, hydrogen coordinates and isotropic and displacement parameters for **3a**.

**Tables 7-11:** Crystallographic data, atomic coordinates, bond lengths, bond angles, anisotropic displacement parameters, hydrogen coordinates and isotropic and displacement parameters for **5c**.

**Table 2.** Crystal data and structure refinement for **3a**.

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Identification code	3a	
Empirical formula	C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>	
Formula weight	201.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 3.9990(4) Å	$\alpha = 71.924(5)^\circ$
	b = 11.1539(11) Å	$\beta = 89.510(8)^\circ$
	c = 12.2250(10) Å	$\gamma = 81.010(5)^\circ$
Volume	511.55(8) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.306 Mg/m <sup>3</sup>	
Absorption coefficient	0.090 mm <sup>-1</sup>	
F(000)	212	
Crystal size	0.34 x 0.11 x 0.06 mm <sup>3</sup>	
Theta range for data collection	3.89 to 25.00°.	
Index ranges	-4<=h<=4, -13<=k<=13, -14<=l<=14	
Reflections collected	2965	
Independent reflections	1765 [R(int) = 0.0272]	
Completeness to theta = 25.00°	97.5 %	
Absorption correction	None	
Max. and min. transmission	0.9945 and 0.9701	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	1765 / 0 / 138	
Goodness-of-fit on F <sup>2</sup>	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1200	
R indices (all data)	R1 = 0.0638, wR2 = 0.1322	
Largest diff. peak and hole	0.215 and -0.259 e.Å <sup>-3</sup>	

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**Table 3.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 3a.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
C(1)	4858(6)	732(2)	1275(2)	32(1)
C(2)	3279(5)	2786(2)	-74(2)	25(1)
C(3)	1427(5)	3524(2)	-1188(2)	24(1)
N(1)	-1611(5)	2222(2)	-2168(2)	34(1)
C(5)	1481(5)	4791(2)	-1612(2)	24(1)
C(6)	98(5)	5734(2)	-2692(2)	24(1)
C(7)	-1471(5)	5464(2)	-3592(2)	27(1)
C(8)	-2610(5)	6428(2)	-4598(2)	28(1)
C(9)	-2264(5)	7695(2)	-4753(2)	25(1)
C(10)	-700(5)	7963(2)	-3860(2)	27(1)
C(11)	474(5)	7004(2)	-2851(2)	26(1)
C(12)	-3525(5)	8729(2)	-5853(2)	31(1)
C(4)	-238(5)	2806(2)	-1743(2)	26(1)
O(1)	2973(3)	1544(1)	233(1)	28(1)
O(2)	4892(4)	3239(1)	481(1)	33(1)

**Table 4.** Bond lengths [Å] and angles [°] for **3a**.

C(1)-O(1)	1.449(2)	O(2)-C(2)-C(3)	124.37(17)
C(1)-H(1A)	0.9800	O(1)-C(2)-C(3)	111.59(16)
C(1)-H(1B)	0.9800	C(5)-C(3)-C(4)	124.99(18)
C(1)-H(1C)	0.9800	C(5)-C(3)-C(2)	118.80(17)
C(2)-O(2)	1.206(2)	C(4)-C(3)-C(2)	116.19(16)
C(2)-O(1)	1.343(2)	C(3)-C(5)-C(6)	131.20(19)
C(2)-C(3)	1.488(3)	C(3)-C(5)-H(5)	114.4
C(3)-C(5)	1.349(3)	C(6)-C(5)-H(5)	114.4
C(3)-C(4)	1.435(3)	C(11)-C(6)-C(7)	117.86(17)
N(1)-C(4)	1.149(3)	C(11)-C(6)-C(5)	116.85(18)
C(5)-C(6)	1.457(3)	C(7)-C(6)-C(5)	125.26(17)
C(5)-H(5)	0.9500	C(8)-C(7)-C(6)	120.59(18)
C(6)-C(11)	1.401(3)	C(8)-C(7)-H(7)	119.7
C(6)-C(7)	1.405(3)	C(6)-C(7)-H(7)	119.7
C(7)-C(8)	1.383(3)	C(7)-C(8)-C(9)	121.60(19)
C(7)-H(7)	0.9500	C(7)-C(8)-H(8)	119.2
C(8)-C(9)	1.395(3)	C(9)-C(8)-H(8)	119.2
C(8)-H(8)	0.9500	C(10)-C(9)-C(8)	117.80(18)
C(9)-C(10)	1.394(3)	C(10)-C(9)-C(12)	121.52(18)
C(9)-C(12)	1.504(3)	C(8)-C(9)-C(12)	120.68(18)
C(10)-C(11)	1.387(3)	C(11)-C(10)-C(9)	121.20(18)
C(10)-H(10)	0.9500	C(11)-C(10)-H(10)	119.4
C(11)-H(11)	0.9500	C(9)-C(10)-H(10)	119.4
C(12)-H(12A)	0.9800	C(10)-C(11)-C(6)	120.93(18)
C(12)-H(12B)	0.9800	C(10)-C(11)-H(11)	119.5
C(12)-H(12C)	0.9800	C(6)-C(11)-H(11)	119.5
O(1)-C(1)-H(1A)	109.5	C(9)-C(12)-H(12A)	109.5
O(1)-C(1)-H(1B)	109.5	C(9)-C(12)-H(12B)	109.5
H(1A)-C(1)-H(1B)	109.5	H(12A)-C(12)-H(12B)	109.5
O(1)-C(1)-H(1C)	109.5	C(9)-C(12)-H(12C)	109.5
H(1A)-C(1)-H(1C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(1B)-C(1)-H(1C)	109.5	H(12B)-C(12)-H(12C)	109.5
O(2)-C(2)-O(1)	124.03(18)	N(1)-C(4)-C(3)	178.6(2)
		C(2)-O(1)-C(1)	115.60(15)

Symmetry transformations used to generate equivalent atoms:

**Table 5.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 3a. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	40(1)	23(1)	30(1)	-3(1)	-3(1)	-5(1)
C(2)	26(1)	23(1)	26(1)	-8(1)	4(1)	-4(1)
C(3)	26(1)	23(1)	25(1)	-10(1)	4(1)	-5(1)
N(1)	39(1)	27(1)	36(1)	-11(1)	-1(1)	-6(1)
C(5)	26(1)	24(1)	25(1)	-11(1)	4(1)	-5(1)
C(6)	23(1)	23(1)	26(1)	-8(1)	2(1)	-3(1)
C(7)	32(1)	25(1)	29(1)	-12(1)	1(1)	-7(1)
C(8)	30(1)	30(1)	26(1)	-12(1)	-2(1)	-5(1)
C(9)	23(1)	27(1)	26(1)	-9(1)	2(1)	-3(1)
C(10)	30(1)	20(1)	31(1)	-8(1)	0(1)	-4(1)
C(11)	28(1)	25(1)	26(1)	-10(1)	0(1)	-5(1)
C(12)	34(1)	28(1)	28(1)	-8(1)	-2(1)	-1(1)
C(4)	28(1)	22(1)	27(1)	-7(1)	3(1)	-4(1)
O(1)	34(1)	20(1)	27(1)	-4(1)	-2(1)	-6(1)
O(2)	46(1)	25(1)	30(1)	-8(1)	-6(1)	-10(1)

**Table 6.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3a**.

	x	y	z	U(eq)
H(1A)	7292	702	1156	48
H(1B)	4302	-133	1467	48
H(1C)	4254	1078	1909	48
H(5)	2618	5126	-1122	29
H(7)	-1752	4610	-3509	33
H(8)	-3654	6224	-5197	34
H(10)	-434	8819	-3946	32
H(11)	1548	7211	-2258	31
H(12A)	-3951	9556	-5712	46
H(12B)	-5632	8554	-6131	46
H(12C)	-1814	8750	-6435	46

**Table 7.** Crystal data and structure refinement for **5c**.

Identification code	5c	
Empirical formula	C <sub>22</sub> H <sub>26</sub> Cl <sub>4</sub> N <sub>4</sub> O <sub>2</sub> Pt	
Formula weight	715.36	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /c	
Unit cell dimensions	a = 9.3767(6) Å	α = 90°
	b = 20.656(3) Å	β = 92.122(5)°
	c = 6.6342(5) Å	γ = 90°
Volume	1284.0(2) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.850 Mg/m <sup>3</sup>	
Absorption coefficient	5.907 mm <sup>-1</sup>	
F(000)	696	
Crystal size	0.19 x 0.14 x 0.04 mm <sup>3</sup>	
Theta range for data collection	2.39 to 27.51°	
Index ranges	-10 ≤ h ≤ 12, -26 ≤ k ≤ 26, -8 ≤ l ≤ 8	
Reflections collected	15313	
Independent reflections	2916 [R(int) = 0.0493]	
Completeness to theta = 27.51°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7937 and 0.4030	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2916 / 0 / 153	
Goodness-of-fit on F <sup>2</sup>	1.074	
Final R indices [I > 2σ(I)]	R1 = 0.0275, wR2 = 0.0477	
R indices (all data)	R1 = 0.0507, wR2 = 0.0530	
Largest diff. peak and hole	0.674 and -0.652 e.Å <sup>-3</sup>	

**Table 8.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **5c**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Pt(1)	5000	0	5000	20(1)
Cl(1)	5811(1)	-564(1)	2310(1)	35(1)
Cl(2)	9167(1)	65(1)	7107(2)	44(1)
O(1)	7475(3)	-1247(1)	8583(4)	31(1)
N(1)	5859(3)	-698(1)	6758(4)	22(1)
N(2)	6729(4)	-1742(2)	7279(5)	31(1)
C(1)	6949(4)	-671(2)	7957(5)	26(1)
C(2)	7714(4)	-86(2)	8709(6)	32(1)
C(3)	7695(5)	-1840(2)	5606(6)	37(1)
C(4)	5423(4)	-1390(2)	6617(6)	27(1)
C(5)	4166(4)	-1513(2)	7921(6)	27(1)
C(6)	4323(5)	-1825(2)	9778(6)	28(1)
C(7)	3155(4)	-1920(2)	10958(6)	31(1)
C(8)	1801(4)	-1708(2)	10338(7)	32(1)
C(9)	543(5)	-1809(2)	11661(8)	48(1)
C(10)	1656(5)	-1397(2)	8495(7)	37(1)
C(11)	2828(4)	-1304(2)	7279(6)	33(1)

**Table 9.** Bond lengths [Å] and angles [°] for **5c**.

Pt(1)-N(1)	2.004(3)	Cl(2)-C(2)-H(2B)	110.1
Pt(1)-N(1)#1	2.004(3)	H(2A)-C(2)-H(2B)	108.4
Pt(1)-Cl(1)	2.2849(9)	N(2)-C(3)-H(3A)	109.5
Pt(1)-Cl(1)#1	2.2849(9)	N(2)-C(3)-H(3B)	109.5
Cl(2)-C(2)	1.786(4)	H(3A)-C(3)-H(3B)	109.5
O(1)-C(1)	1.349(5)	N(2)-C(3)-H(3C)	109.5
O(1)-N(2)	1.496(4)	H(3A)-C(3)-H(3C)	109.5
N(1)-C(1)	1.273(5)	H(3B)-C(3)-H(3C)	109.5
N(1)-C(4)	1.489(5)	N(2)-C(4)-N(1)	103.4(3)
N(2)-C(3)	1.473(5)	N(2)-C(4)-C(5)	113.8(3)
N(2)-C(4)	1.477(5)	N(1)-C(4)-C(5)	110.1(3)
C(1)-C(2)	1.483(6)	N(2)-C(4)-H(4)	109.8
C(2)-H(2A)	0.9900	N(1)-C(4)-H(4)	109.8
C(2)-H(2B)	0.9900	C(5)-C(4)-H(4)	109.8
C(3)-H(3A)	0.9800	C(11)-C(5)-C(6)	118.8(4)
C(3)-H(3B)	0.9800	C(11)-C(5)-C(4)	119.5(3)
C(3)-H(3C)	0.9800	C(6)-C(5)-C(4)	121.7(4)
C(4)-C(5)	1.509(5)	C(7)-C(6)-C(5)	120.4(4)
C(4)-H(4)	1.0000	C(7)-C(6)-H(6)	119.8
C(5)-C(11)	1.379(6)	C(5)-C(6)-H(6)	119.8
C(5)-C(6)	1.395(5)	C(6)-C(7)-C(8)	121.4(4)
C(6)-C(7)	1.383(6)	C(6)-C(7)-H(7)	119.3
C(6)-H(6)	0.9500	C(8)-C(7)-H(7)	119.3
C(7)-C(8)	1.391(6)	C(10)-C(8)-C(7)	117.8(4)
C(7)-H(7)	0.9500	C(10)-C(8)-C(9)	121.7(4)
C(8)-C(10)	1.383(6)	C(7)-C(8)-C(9)	120.6(4)
C(8)-C(9)	1.511(6)	C(8)-C(9)-H(9A)	109.5
C(9)-H(9A)	0.9800	C(8)-C(9)-H(9B)	109.5
C(9)-H(9B)	0.9800	H(9A)-C(9)-H(9B)	109.5
C(9)-H(9C)	0.9800	C(8)-C(9)-H(9C)	109.5
C(10)-C(11)	1.400(6)	H(9A)-C(9)-H(9C)	109.5
C(10)-H(10)	0.9500	H(9B)-C(9)-H(9C)	109.5
C(11)-H(11)	0.9500	C(8)-C(10)-C(11)	121.3(4)
		C(8)-C(10)-H(10)	119.4
N(1)-Pt(1)-N(1)#1	180.00(12)	C(11)-C(10)-H(10)	119.4
N(1)-Pt(1)-Cl(1)	87.10(8)	C(5)-C(11)-C(10)	120.3(4)
N(1)#1-Pt(1)-Cl(1)	92.90(8)	C(5)-C(11)-H(11)	119.9
N(1)-Pt(1)-Cl(1)#1	92.90(8)	C(10)-C(11)-H(11)	119.9
N(1)#1-Pt(1)-Cl(1)#1	87.10(8)		
Cl(1)-Pt(1)-Cl(1)#1	180.0		
C(1)-O(1)-N(2)	105.4(3)		
C(1)-N(1)-C(4)	107.1(3)		
C(1)-N(1)-Pt(1)	128.9(3)		
C(4)-N(1)-Pt(1)	123.4(2)		
C(3)-N(2)-C(4)	111.8(3)		
C(3)-N(2)-O(1)	104.0(3)		
C(4)-N(2)-O(1)	101.6(3)		
N(1)-C(1)-O(1)	115.5(3)		
N(1)-C(1)-C(2)	127.8(4)		
O(1)-C(1)-C(2)	116.7(3)		
C(1)-C(2)-Cl(2)	108.2(3)		
C(1)-C(2)-H(2A)	110.1		
Cl(2)-C(2)-H(2A)	110.1		
C(1)-C(2)-H(2B)	110.1		

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Symmetry transformations used to generate equivalent atoms:

#1  $-x+1,-y,-z+1$

**Table 10.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5c. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^2 U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Pt(1)	26(1)	16(1)	17(1)	-1(1)	3(1)	-1(1)
Cl(1)	56(1)	28(1)	21(1)	-3(1)	12(1)	9(1)
Cl(2)	40(1)	45(1)	46(1)	-1(1)	12(1)	-13(1)
O(1)	33(2)	28(2)	31(2)	0(1)	-2(1)	7(1)
N(1)	27(2)	19(2)	19(2)	-1(1)	4(1)	0(1)
N(2)	33(2)	24(2)	36(2)	-3(2)	1(2)	4(2)
C(1)	32(2)	26(2)	21(2)	0(2)	8(2)	1(2)
C(2)	35(2)	30(3)	30(2)	-1(2)	4(2)	0(2)
C(3)	38(3)	33(2)	42(3)	-6(2)	10(2)	5(2)
C(4)	39(2)	18(2)	24(2)	-1(2)	0(2)	1(2)
C(5)	35(2)	16(2)	29(2)	1(2)	1(2)	-2(2)
C(6)	29(2)	25(2)	31(2)	-1(2)	-2(2)	1(2)
C(7)	39(2)	23(2)	33(2)	3(2)	4(2)	0(2)
C(8)	35(2)	16(2)	45(3)	0(2)	8(2)	-6(2)
C(9)	40(3)	34(3)	69(3)	8(2)	13(3)	-8(2)
C(10)	27(2)	27(2)	56(3)	8(2)	-8(2)	-3(2)
C(11)	39(2)	21(2)	38(2)	10(2)	-7(2)	-4(2)

**Table 11.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **5c**.

	x	y	z	U(eq)
H(2A)	8076	-155	10113	38
H(2B)	7059	290	8692	38
H(3A)	7291	-2167	4678	56
H(3B)	8627	-1988	6144	56
H(3C)	7812	-1431	4881	56
H(4)	5163	-1502	5184	33
H(6)	5237	-1974	10237	34
H(7)	3281	-2135	12218	38
H(9A)	626	-1519	12828	71
H(9B)	530	-2260	12127	71
H(9C)	-343	-1715	10887	71
H(10)	744	-1244	8045	45
H(11)	2701	-1097	6007	39

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