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cis-Diammine[3-(3-chloro-7-methoxy-9,10-dihydroacridin-9-ylideneamino)propan-1-amine- κ^2N,N']platinum(II) dinitrate

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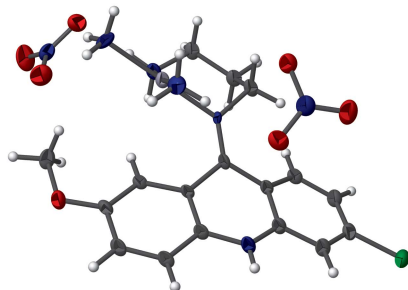
Keywords: crystal structure; platinum ammine complex; 9-aminoacridine; 9,10-dihydroacridin-9-imine.

CCDC reference: 1469909

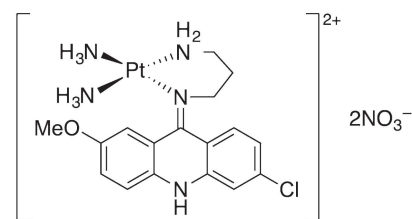
Structural data: full structural data are available from iucrdata.iucr.org

The title complex salt, $[\text{Pt}(\text{C}_{16}\text{H}_{17}\text{N}_3)(\text{NH}_3)_2](\text{NO}_3)_2$, is of interest with respect to anticancer activity. The secondary amine of 9-aminoacridine coordinates with the platinum(II) atom, leading to imine–platinum complex cation formation. The crystal structure displays extensive $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonding and weak $\text{C}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding.

3D view



Chemical scheme



Structure description

Platinum has been widely used for chemotherapy since cisplatin was approved by the US Food and Drug Administration in 1978 (Galanski *et al.*, 2005). Unfortunately, due to the widespread use of platinum drugs, patients began to develop drug resistance (Shen *et al.*, 2012). Non-classical platinum drugs, for example, platinum-intercalator conjugates are thought to be an alternative solution to overcome cisplatin resistance (Johnstone *et al.*, 2014; Baruah *et al.*, 2004; Martins *et al.*, 2001). We attempted to synthesize a 9-aminoacridine derivative linked with monofunctional platinum *via* a three-carbon alkyl chain. During the platination reaction between the primary amine and *cis*- $[\text{Pt}(\text{NH}_3)_2(\text{O-donor})\text{Cl}]^+$ (O-donor = *OI*-DMF and NO_3^-), an unexpected product formed predominantly. We grew crystals of the compound to investigate the structure *via* X-ray diffraction of the crystal.

The secondary amine of 9-aminoacridine replaced the chloride to form a platinum–nitrogen complex. The platinum complex (Fig. 1) has a square-planar geometry and the three-carbon alkyl chain became part of a newly formed six-membered ring with Pt, N13 and N9. The longer bond lengths of N13–Pt [2.053 (9) Å] and N9–Pt [1.993 (8) Å] appears to compensate for the smaller bond angle of N13–Pt–N9 [87.3 (3)°], allowing the six-membered ring to adopt a conformation similar to a chair conformation. The bond

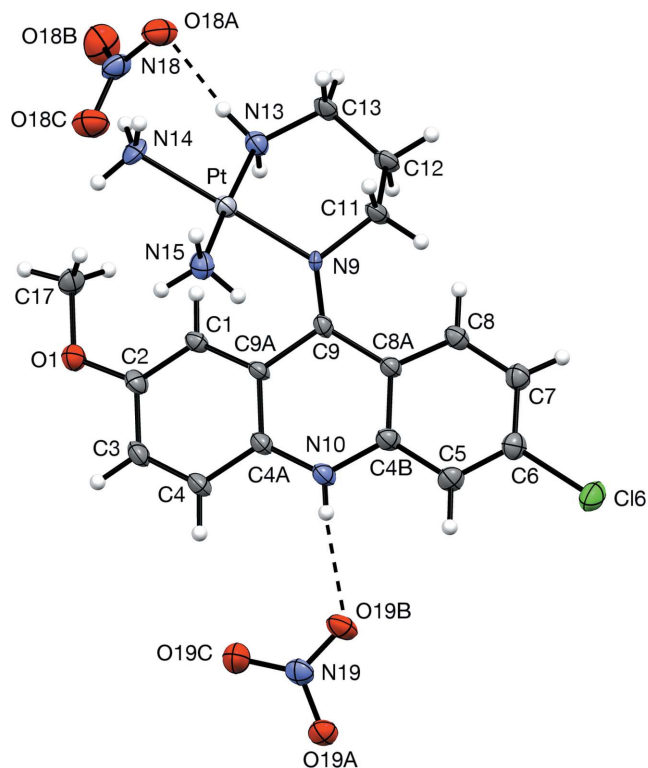


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids for the non-H atoms at the 50% probability level.

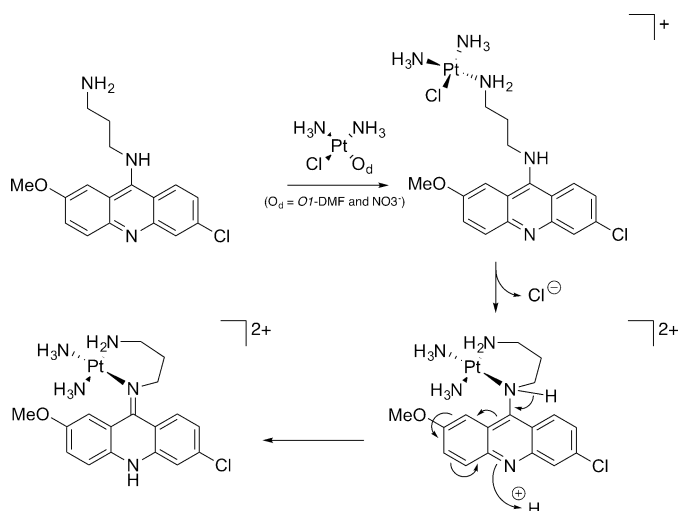


Figure 2
Potential mechanism of the formation of the title compound.

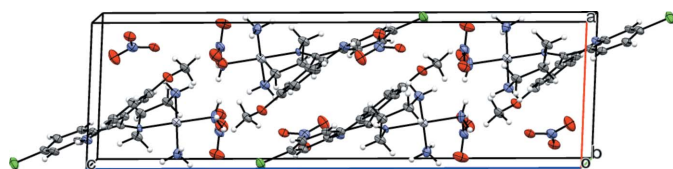


Figure 3
Packing plot of the title compound.

Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N10—H10···O19B ⁱ	0.72 (12)	2.20 (12)	2.919 (12)	172 (14)
N13—H13C···O19A ⁱⁱ	0.91	2.06	2.910 (13)	155
N13—H13D···N18	0.91	2.63	3.428 (13)	147
N13—H13D···O18A	0.91	2.03	2.918 (13)	166
N14—H14A···O18A ⁱⁱⁱ	0.91	2.24	3.113 (14)	160
N14—H14B···O18C	0.91	2.43	3.218 (15)	146
N14—H14C···O18B ^{iv}	0.91	2.54	3.294 (15)	140
N14—H14C···Cl6 ^v	0.91	2.82	3.497 (10)	132
N15—H15A···O18C ^{iv}	0.91	2.38	3.257 (15)	162
N15—H15B···O19A	0.91	2.52	3.120 (13)	124
N15—H15B···O19B	0.91	2.27	3.183 (13)	178
N15—H15C···O18B ⁱⁱⁱ	0.91	2.48	3.223 (14)	139
N15—H15C···O18A ⁱⁱⁱ	0.91	2.40	3.192 (13)	146
C4—H4···O19C ⁱ	0.95	2.46	3.354 (14)	157
C7—H7···O19A ^{vi}	0.95	2.64	3.576 (14)	170
C11—H11B···Cl6 ^{vi}	0.99	2.95	3.649 (12)	128
C17—H17A···O18A ⁱⁱⁱ	0.98	2.54	3.250 (15)	129
C17—H17B···O18B ^{vii}	0.98	2.45	3.356 (15)	154
C17—H17C···O19A ⁱⁱ	0.98	2.63	3.568 (14)	160

Symmetry codes: (i) $-x + 2, -y + 1, -z + 1$; (ii) $x - 1, y, z$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (iv) $x + 1, y, z$; (v) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (vi) $-x + 2, -y + 2, -z + 1$; (vii) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.

length of N9—C9 [1.293 (13) Å], 120° bond angles around N9 and C9, and the protonation of N10 suggest the formation of an imine and proton rearrangement (Fig. 2). The resulting acridin-imine is strained around C9. The C1—C9A—C9—N9 torsion angle is 33 (1)° and C8—C8A—C9—N9 is −35 (2)°.

Table 2
Experimental details.

Crystal data	[Pt(C ₁₆ H ₁₈ N ₃)(NH ₃) ₂](NO ₃) ₂
Chemical formula	668.97
<i>M_r</i>	Monoclinic, <i>P</i> ₂ /c
Crystal system, space group	100
Temperature (K)	7.6398 (3), 10.8372 (11), 25.982 (4)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	92.478 (5)
β (°)	2149.1 (4)
<i>V</i> (Å ³)	4
<i>Z</i>	Cu Kα
Radiation type	13.87
μ (mm ^{−1})	0.13 × 0.02 × 0.02
Crystal size (mm)	
Data collection	
Diffractometer	Agilent SuperNova with AtlasS2 CCD
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Agilent, 2013)
<i>T</i> _{min} , <i>T</i> _{max}	0.503, 1.00
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	8178, 4158, 3105
<i>R</i> _{int}	0.066
(sin θ/λ) _{max} (Å ^{−1})	0.627
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.059, 0.155, 1.04
No. of reflections	4158
No. of parameters	304
No. of restraints	444
H-atom treatment	Only H-atom coordinates refined
Δρ _{max} , Δρ _{min} (e Å ^{−3})	2.22, −3.37

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXL2014* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

The ring is bent approximately 15° , resembling a bow when viewed from the side.

There are two nitrate ions present in the crystal. One nitrate can form hydrogen bonds (Table 1) with H10 [H10—O19B = 2.20 (12) Å] and H13C (H13C—O19A = 2.059 Å), and the other can form a hydrogen bond with H13D (H13D—O18A = 2.03 Å). The packing is illustrated in Fig. 3.

Synthesis and crystallization

cis-[Pt(NH₃)₂(O_d)Cl]⁺ (O_d = *OI*-DMF and NO₃[−]) was prepared from cisplatin (45 mg, 0.15 mmol) and silver nitrate (26 mg, 0.15 mmol) in *N,N*-dimethylformamide at 55°C in the dark for 1–3 days (Hollis *et al.*, 1989). The title compound was prepared by mixing *N*¹-(6-chloro-2-methoxyacridin-9-yl)propane-1,3-diamine (32 mg, 0.1 mmol) and *cis*-[Pt(NH₃)₂(O_d)Cl]⁺ in DMF at 55°C in the dark for 24 h. DMF was removed under high vacuum and the crude mixture was dissolved in methanol (4 ml). Any undissolved solids were removed *via* filtration. Cold diethyl ether (60 ml) was poured to the filtrate, resulting in precipitation of the desired product. The fine precipitates were collected with EMD Millipore HNWP grade 0.45 μm nylon membrane filter (37 mg, 0.042 mmol, 42% yield). Yellow, thin-needle crystals of the title compound were obtained from vapor diffusion between methanol and diethyl ether.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

- Agilent (2013). *CrysAlis PRO*. Agilent Technologies UK Ltd, Oxfordshire, England.
- Baruah, H., Barry, C. G. & Bierbach, U. (2004). *Curr. Top. Med. Chem.* **4**, 1537–1549.
- Galanski, M., Jakupec, M. A. & Keppler, B. K. (2005). *Curr. Med. Chem.* **12**, 2075–2094.
- Hollis, L. S., Amundsen, A. R. & Stern, E. W. (1989). *J. Med. Chem.* **32**, 128–136.
- Johnstone, T. C., Park, G. Y. & Lippard, S. J. (2014). *Anticancer Res.* **34**, 471–476.
- Martins, E. T., Baruah, H., Kramarczyk, J., Saluta, G., Day, C. S., Kucera, G. L. & Bierbach, U. (2001). *J. Med. Chem.* **44**, 4492–4496.
- Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst. C* **71**, 3–8.
- Shen, D.-W., Pouliot, L. M., Hall, M. D. & Gottesman, M. M. (2012). *Pharmacol. Rev.* **64**, 706–721.

full crystallographic data

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***cis*-Diammine[3-(3-chloro-7-methoxy-9,10-dihydroacridin-9-ylideneamino)-propan-1-amine- κ^2 N,N']platinum(II) dinitrate**

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cis-Diammine[3-(3-chloro-7-methoxy-9,10-dihydroacridin-9-ylideneamino)propan-1-amine- κ^2 N,N']platinum(II) dinitrate

Crystal data

[Pt(C₁₆H₁₈N₃)(NH₃)₂](NO₃)₂

$M_r = 668.97$

Monoclinic, $P2_1/c$

$a = 7.6398$ (3) Å

$b = 10.8372$ (11) Å

$c = 25.982$ (4) Å

$\beta = 92.478$ (5)°

$V = 2149.1$ (4) Å³

$Z = 4$

$F(000) = 1304$

$D_x = 2.068$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 2416 reflections

$\theta = 3.4\text{--}72.7^\circ$

$\mu = 13.87$ mm⁻¹

$T = 100$ K

Needle, yellow

$0.13 \times 0.02 \times 0.02$ mm

Data collection

Agilent SuperNova with AtlasS2 CCD diffractometer

Radiation source: sealed microfocus tube

ω -scans

Absorption correction: gaussian

(*CrysAlis PRO*; Agilent, 2013)

$T_{\min} = 0.503$, $T_{\max} = 1.00$

8178 measured reflections

4158 independent reflections

3105 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

$\theta_{\max} = 75.2^\circ$, $\theta_{\min} = 3.4^\circ$

$h = -9 \rightarrow 5$

$k = -13 \rightarrow 7$

$l = -30 \rightarrow 31$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.155$

$S = 1.04$

4158 reflections

304 parameters

444 restraints

Hydrogen site location: inferred from neighbouring sites

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 7.5338P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 2.22$ e Å⁻³

$\Delta\rho_{\min} = -3.37$ e Å⁻³

Special details

Geometry. 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C13	0.5794 (15)	1.0413 (10)	0.6474 (4)	0.024 (2)
H13A	0.6710	1.0710	0.6725	0.028*
H13B	0.4831	1.1025	0.6463	0.028*
C12	0.6562 (15)	1.0332 (10)	0.5942 (4)	0.024 (2)
H12A	0.5618	1.0093	0.5689	0.029*
H12B	0.6978	1.1162	0.5845	0.029*
C11	0.8071 (15)	0.9424 (10)	0.5904 (5)	0.025 (2)
H11A	0.8578	0.9494	0.5561	0.029*
H11B	0.9000	0.9621	0.6169	0.029*
C9	0.7168 (13)	0.7372 (9)	0.5604 (4)	0.0181 (18)
C8A	0.7632 (13)	0.7546 (9)	0.5058 (4)	0.0187 (19)
C8	0.7575 (13)	0.8684 (10)	0.4799 (4)	0.022 (2)
H8	0.7111	0.9386	0.4965	0.026*
C7	0.8178 (14)	0.8798 (11)	0.4312 (4)	0.026 (2)
H7	0.8093	0.9563	0.4135	0.031*
C6	0.8915 (14)	0.7780 (11)	0.4084 (4)	0.025 (2)
C5	0.8907 (13)	0.6629 (11)	0.4302 (4)	0.024 (2)
H5	0.9377	0.5937	0.4131	0.029*
C4B	0.8181 (13)	0.6505 (10)	0.4788 (4)	0.022 (2)
C4A	0.7001 (14)	0.5117 (10)	0.5402 (4)	0.020 (2)
C4	0.6508 (14)	0.3901 (10)	0.5529 (4)	0.023 (2)
H4	0.6940	0.3219	0.5343	0.027*
C3	0.5401 (15)	0.3714 (11)	0.5923 (4)	0.025 (2)
H3	0.5032	0.2900	0.5998	0.030*
C2	0.4806 (14)	0.4694 (10)	0.6216 (4)	0.024 (2)
C1	0.5295 (13)	0.5870 (9)	0.6094 (4)	0.0181 (19)
H1	0.4828	0.6545	0.6277	0.022*
C9A	0.6466 (13)	0.6103 (9)	0.5707 (4)	0.0180 (19)
C17	0.3137 (15)	0.5425 (11)	0.6906 (4)	0.028 (2)
H17A	0.4163	0.5799	0.7083	0.042*
H17B	0.2330	0.5124	0.7161	0.042*
H17C	0.2542	0.6042	0.6685	0.042*
N13	0.5114 (12)	0.9219 (8)	0.6653 (4)	0.0247 (19)
H13C	0.4258	0.8952	0.6425	0.030*
H13D	0.4625	0.9330	0.6963	0.030*
N9	0.7426 (10)	0.8136 (7)	0.5982 (3)	0.0131 (15)
N10	0.8018 (12)	0.5329 (9)	0.4987 (4)	0.0224 (19)
N15	0.9092 (13)	0.6683 (9)	0.6799 (4)	0.028 (2)
H15A	0.9869	0.6955	0.7049	0.042*
H15B	0.9632	0.6636	0.6494	0.042*
H15C	0.8693	0.5923	0.6885	0.042*
N14	0.6630 (14)	0.7624 (9)	0.7488 (3)	0.030 (2)
H14A	0.6614	0.6801	0.7557	0.045*
H14B	0.5588	0.7965	0.7569	0.045*
H14C	0.7512	0.7988	0.7680	0.045*

N18	0.1917 (13)	0.8899 (10)	0.7529 (4)	0.031 (2)
N19	1.1839 (13)	0.7603 (9)	0.5780 (4)	0.0285 (19)
O1	0.3694 (10)	0.4397 (7)	0.6591 (3)	0.0281 (17)
O18C	0.2424 (13)	0.7816 (9)	0.7465 (4)	0.046 (2)
O18B	0.0363 (12)	0.9147 (10)	0.7567 (4)	0.052 (3)
O18A	0.3072 (12)	0.9761 (9)	0.7549 (4)	0.039 (2)
O19A	1.1896 (10)	0.8149 (7)	0.6210 (3)	0.0280 (17)
O19B	1.1044 (11)	0.6585 (7)	0.5742 (3)	0.0304 (18)
O19C	1.2554 (14)	0.8075 (8)	0.5413 (4)	0.047 (2)
Cl6	0.9803 (4)	0.7921 (3)	0.34724 (11)	0.0360 (7)
Pt	0.70226 (6)	0.78889 (4)	0.67275 (2)	0.02123 (16)
H10	0.816 (17)	0.483 (12)	0.481 (5)	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C13	0.025 (4)	0.013 (4)	0.034 (5)	0.005 (3)	0.009 (4)	0.002 (3)
C12	0.027 (4)	0.013 (4)	0.033 (5)	0.004 (4)	0.008 (4)	-0.001 (3)
C11	0.025 (4)	0.012 (4)	0.037 (5)	0.000 (3)	0.012 (4)	-0.002 (3)
C9	0.017 (4)	0.014 (3)	0.024 (3)	-0.002 (3)	0.005 (3)	0.003 (3)
C8A	0.018 (4)	0.014 (3)	0.024 (3)	-0.001 (3)	0.005 (3)	-0.001 (3)
C8	0.019 (4)	0.017 (4)	0.029 (4)	0.001 (3)	0.002 (3)	0.000 (3)
C7	0.025 (5)	0.024 (4)	0.028 (4)	0.000 (4)	0.005 (3)	0.002 (3)
C6	0.020 (4)	0.027 (4)	0.029 (4)	-0.004 (3)	0.007 (3)	0.000 (3)
C5	0.018 (4)	0.024 (4)	0.030 (4)	0.003 (3)	0.007 (3)	-0.001 (3)
C4B	0.019 (4)	0.018 (4)	0.029 (4)	0.000 (3)	0.007 (3)	-0.002 (3)
C4A	0.022 (4)	0.014 (3)	0.026 (4)	-0.002 (3)	0.002 (3)	0.001 (3)
C4	0.024 (4)	0.013 (4)	0.031 (4)	-0.002 (3)	0.002 (4)	0.001 (3)
C3	0.029 (4)	0.015 (4)	0.032 (4)	-0.005 (3)	0.004 (4)	0.003 (3)
C2	0.025 (4)	0.018 (4)	0.029 (4)	-0.008 (3)	0.004 (4)	-0.002 (3)
C1	0.015 (4)	0.014 (4)	0.024 (4)	0.001 (3)	0.001 (3)	-0.001 (3)
C9A	0.019 (4)	0.010 (3)	0.025 (4)	-0.002 (3)	0.004 (3)	-0.002 (3)
C17	0.028 (5)	0.027 (5)	0.031 (5)	0.006 (4)	0.011 (4)	0.002 (4)
N13	0.027 (4)	0.019 (4)	0.029 (4)	-0.002 (3)	0.005 (3)	0.001 (3)
N9	0.016 (3)	0.012 (3)	0.011 (3)	-0.003 (3)	0.004 (2)	0.003 (2)
N10	0.022 (4)	0.015 (3)	0.031 (4)	-0.002 (3)	0.008 (3)	-0.001 (3)
N15	0.034 (4)	0.025 (5)	0.025 (5)	0.000 (4)	0.000 (4)	0.005 (4)
N14	0.045 (5)	0.033 (5)	0.012 (4)	0.001 (4)	0.002 (3)	-0.001 (3)
N18	0.029 (4)	0.036 (4)	0.028 (5)	0.003 (3)	0.011 (3)	-0.006 (3)
N19	0.029 (4)	0.022 (4)	0.035 (4)	0.007 (3)	0.005 (3)	0.001 (3)
O1	0.030 (4)	0.023 (4)	0.033 (4)	-0.004 (3)	0.012 (3)	0.000 (3)
O18C	0.051 (5)	0.036 (4)	0.051 (6)	0.006 (4)	0.013 (4)	-0.010 (4)
O18B	0.031 (4)	0.054 (6)	0.072 (7)	0.004 (4)	0.017 (4)	0.006 (5)
O18A	0.037 (4)	0.037 (4)	0.046 (5)	-0.005 (3)	0.012 (4)	-0.014 (4)
O19A	0.023 (4)	0.026 (4)	0.035 (4)	0.005 (3)	0.007 (3)	-0.002 (3)
O19B	0.029 (4)	0.019 (3)	0.044 (5)	0.004 (3)	0.006 (3)	-0.004 (3)
O19C	0.065 (6)	0.032 (5)	0.044 (4)	-0.004 (4)	0.025 (4)	0.001 (4)
Cl6	0.0408 (15)	0.0412 (17)	0.0271 (14)	-0.0127 (15)	0.0124 (12)	-0.0027 (13)

Pt 0.0231 (2) 0.0156 (2) 0.0255 (3) 0.0002 (2) 0.00693 (17) 0.0003 (2)

Geometric parameters (Å, °)

C13—H13A	0.9900	C3—H3	0.9500
C13—H13B	0.9900	C3—C2	1.393 (16)
C13—C12	1.527 (14)	C2—C1	1.370 (15)
C13—N13	1.477 (13)	C2—O1	1.359 (13)
C12—H12A	0.9900	C1—H1	0.9500
C12—H12B	0.9900	C1—C9A	1.398 (13)
C12—C11	1.522 (14)	C17—H17A	0.9800
C11—H11A	0.9900	C17—H17B	0.9800
C11—H11B	0.9900	C17—H17C	0.9800
C11—N9	1.497 (12)	C17—O1	1.457 (13)
C9—C8A	1.489 (14)	N13—H13C	0.9100
C9—C9A	1.504 (14)	N13—H13D	0.9100
C9—N9	1.293 (13)	N13—Pt	2.053 (9)
C8A—C8	1.404 (15)	N9—Pt	1.993 (8)
C8A—C4B	1.402 (14)	N10—H10	0.72 (12)
C8—H8	0.9500	N15—H15A	0.9100
C8—C7	1.371 (14)	N15—H15B	0.9100
C7—H7	0.9500	N15—H15C	0.9100
C7—C6	1.384 (16)	N15—Pt	2.053 (10)
C6—C5	1.371 (16)	N14—H14A	0.9100
C6—C16	1.760 (11)	N14—H14B	0.9100
C5—H5	0.9500	N14—H14C	0.9100
C5—C4B	1.407 (14)	N14—Pt	2.033 (9)
C4B—N10	1.383 (14)	N18—O18C	1.249 (13)
C4A—C4	1.414 (14)	N18—O18B	1.225 (13)
C4A—C9A	1.402 (14)	N18—O18A	1.284 (13)
C4A—N10	1.374 (14)	N19—O19A	1.262 (12)
C4—H4	0.9500	N19—O19B	1.261 (13)
C4—C3	1.370 (15)	N19—O19C	1.231 (13)
H13A—C13—H13B	107.8	O1—C2—C1	124.8 (10)
C12—C13—H13A	109.0	C2—C1—H1	119.2
C12—C13—H13B	109.0	C2—C1—C9A	121.6 (10)
N13—C13—H13A	109.0	C9A—C1—H1	119.2
N13—C13—H13B	109.0	C4A—C9A—C9	118.8 (9)
N13—C13—C12	112.9 (9)	C1—C9A—C9	122.4 (9)
C13—C12—H12A	108.6	C1—C9A—C4A	118.8 (9)
C13—C12—H12B	108.6	H17A—C17—H17B	109.5
H12A—C12—H12B	107.6	H17A—C17—H17C	109.5
C11—C12—C13	114.7 (9)	H17B—C17—H17C	109.5
C11—C12—H12A	108.6	O1—C17—H17A	109.5
C11—C12—H12B	108.6	O1—C17—H17B	109.5
C12—C11—H11A	109.7	O1—C17—H17C	109.5
C12—C11—H11B	109.7	C13—N13—H13C	109.0

H11A—C11—H11B	108.2	C13—N13—H13D	109.0
N9—C11—C12	109.8 (9)	C13—N13—Pt	112.8 (7)
N9—C11—H11A	109.7	H13C—N13—H13D	107.8
N9—C11—H11B	109.7	Pt—N13—H13C	109.0
C8A—C9—C9A	112.7 (9)	Pt—N13—H13D	109.0
N9—C9—C8A	127.4 (9)	C11—N9—Pt	108.8 (6)
N9—C9—C9A	119.7 (9)	C9—N9—C11	122.3 (8)
C8—C8A—C9	124.3 (9)	C9—N9—Pt	128.8 (7)
C8—C8A—C4B	118.1 (10)	C4B—N10—H10	115 (10)
C4B—C8A—C9	117.6 (9)	C4A—N10—C4B	120.7 (9)
C8A—C8—H8	119.5	C4A—N10—H10	119 (10)
C7—C8—C8A	121.1 (10)	H15A—N15—H15B	109.5
C7—C8—H8	119.5	H15A—N15—H15C	109.5
C8—C7—H7	120.5	H15B—N15—H15C	109.5
C8—C7—C6	118.9 (11)	Pt—N15—H15A	109.5
C6—C7—H7	120.5	Pt—N15—H15B	109.5
C7—C6—Cl6	119.9 (9)	Pt—N15—H15C	109.5
C5—C6—C7	122.5 (10)	H14A—N14—H14B	109.5
C5—C6—Cl6	117.5 (9)	H14A—N14—H14C	109.5
C6—C5—H5	121.1	H14B—N14—H14C	109.5
C6—C5—C4B	117.9 (10)	Pt—N14—H14A	109.5
C4B—C5—H5	121.1	Pt—N14—H14B	109.5
C8A—C4B—C5	120.7 (10)	Pt—N14—H14C	109.5
N10—C4B—C8A	121.3 (10)	O18C—N18—O18A	118.2 (10)
N10—C4B—C5	117.9 (10)	O18B—N18—O18C	121.6 (11)
C9A—C4A—C4	119.3 (10)	O18B—N18—O18A	120.2 (11)
N10—C4A—C4	120.3 (10)	O19B—N19—O19A	118.6 (10)
N10—C4A—C9A	120.3 (9)	O19C—N19—O19A	119.3 (10)
C4A—C4—H4	120.3	O19C—N19—O19B	122.0 (11)
C3—C4—C4A	119.5 (10)	C2—O1—C17	115.4 (9)
C3—C4—H4	120.3	N9—Pt—N13	87.3 (3)
C4—C3—H3	119.3	N9—Pt—N15	91.3 (4)
C4—C3—C2	121.5 (10)	N9—Pt—N14	179.5 (4)
C2—C3—H3	119.3	N15—Pt—N13	174.9 (4)
C1—C2—C3	119.0 (10)	N14—Pt—N13	93.3 (4)
O1—C2—C3	116.1 (10)	N14—Pt—N15	88.2 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N10—H10...O19B ⁱ	0.72 (12)	2.20 (12)	2.919 (12)	172 (14)
N13—H13C...O19A ⁱⁱ	0.91	2.06	2.910 (13)	155
N13—H13D...N18	0.91	2.63	3.428 (13)	147
N13—H13D...O18A	0.91	2.03	2.918 (13)	166
N14—H14A...O18A ⁱⁱⁱ	0.91	2.24	3.113 (14)	160
N14—H14B...O18C	0.91	2.43	3.218 (15)	146
N14—H14C...O18B ^{iv}	0.91	2.54	3.294 (15)	140
N14—H14C...Cl6 ^v	0.91	2.82	3.497 (10)	132

N15—H15A···O18C ^{iv}	0.91	2.38	3.257 (15)	162
N15—H15B···O19A	0.91	2.52	3.120 (13)	124
N15—H15B···O19B	0.91	2.27	3.183 (13)	178
N15—H15C···O18B ⁱⁱⁱ	0.91	2.48	3.223 (14)	139
N15—H15C···O18A ⁱⁱⁱ	0.91	2.40	3.192 (13)	146
C4—H4···O19C ⁱ	0.95	2.46	3.354 (14)	157
C7—H7···O19A ^{vi}	0.95	2.64	3.576 (14)	170
C11—H11B···C16 ^{vi}	0.99	2.95	3.649 (12)	128
C17—H17A···O18A ⁱⁱⁱ	0.98	2.54	3.250 (15)	129
C17—H17B···O18B ^{vii}	0.98	2.45	3.356 (15)	154
C17—H17C···O19A ⁱⁱ	0.98	2.63	3.568 (14)	160

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+1, y-1/2, -z+3/2$; (iv) $x+1, y, z$; (v) $x, -y+3/2, z+1/2$; (vi) $-x+2, -y+2, -z+1$; (vii) $-x, y-1/2, -z+3/2$.