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

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The title complex salt, $[Pt(C_{16}H_{17}N_3)(NH_3)_2](NO_3)_2$, 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 $N-H\cdots O$ and $N-H\cdots N$ hydrogen bonding and weak $C-H\cdots Cl$ and $C-H\cdots O$ hydrogen bonding.



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-amino-acridine derivative linked with monofunctional platinum *via* a three-carbon alkyl chain. During the platination reaction between the primary amine and *cis*-[Pt(NH₃)₂(O-donor)Cl]⁺ (O-donor = *O1*-DMF and NO₃⁻), 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 platinumnitrogen 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





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

Table 2

Crystal data

 $\Delta \rho_{\rm max}, \, \Delta \rho_{\rm min} \ ({\rm e} \ {\rm \AA}^{-3})$

Experimental details.

, , ,	2 ())			
$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
N10-H10···O19 B^{i}	0.72 (12)	2.20 (12)	2.919 (12)	172 (14)
N13-H13 $C \cdots$ O19 A^{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 $-$ H14 A \cdots O18 A ⁱⁱⁱ	0.91	2.24	3.113 (14)	160
$N14-H14B\cdots O18C$	0.91	2.43	3.218 (15)	146
N14 $-$ H14 C ···O18 B ^{iv}	0.91	2.54	3.294 (15)	140
$N14-H14C\cdots Cl6^{v}$	0.91	2.82	3.497 (10)	132
N15-H15 A ···O18 C ^{iv}	0.91	2.38	3.257 (15)	162
$N15-H15B\cdots O19A$	0.91	2.52	3.120 (13)	124
$N15-H15B\cdots O19B$	0.91	2.27	3.183 (13)	178
$N15-H15C \cdot \cdot \cdot O18B^{iii}$	0.91	2.48	3.223 (14)	139
$N15-H15C\cdots O18A^{iii}$	0.91	2.40	3.192 (13)	146
$C4-H4\cdots O19C^{i}$	0.95	2.46	3.354 (14)	157
$C7-H7\cdots O19A^{vi}$	0.95	2.64	3.576 (14)	170
$C11 - H11B \cdots Cl6^{vi}$	0.99	2.95	3.649 (12)	128
$C17-H17A\cdots O18A^{iii}$	0.98	2.54	3.250 (15)	129
$C17 - H17B \cdots O18B^{vii}$	0.98	2.45	3.356 (15)	154
$C17-H17C\cdots O19A^{ii}$	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 $-35 (2)^{\circ}$.

Figure 1

The molecular structure of the title compound, showing the atomnumbering 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.

Ci ystai uata	
Chemical formula	$[Pt(C_{16}H_{18}N_3)(NH_3)_2](NO_3)_2$
$M_{\rm r}$	668.97
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.6398 (3), 10.8372 (11), 25.982 (4)
β (°)	92.478 (5)
$V(\dot{A}^3)$	2149.1 (4)
Ζ	4
Radiation type	Cu Ka
$\mu \text{ (mm}^{-1})$	13.87
Crystal size (mm)	$0.13 \times 0.02 \times 0.02$
Data collection	
Diffractometer	Agilent SuperNova with AtlasS2 CCD
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Agilent, 2013)
<i>T</i>	0.503. 1.00
No. of measured, independent and	8178, 4158, 3105
observed $[I > 2\sigma(I)]$ reflections	
Rint	0.066
$(\sin \theta / \lambda)_{\max} (\text{\AA}^{-1})$	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)] w R(F^2) S$	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

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

2.22, -3.37

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 = O1-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- $[Pt(NH_3)_2(O_d)Cl]^+$ 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 nvlon 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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full crystallographic data

IUCrData (2016). **1**, x160481 [doi:10.1107/S2414314616004818]

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

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

F(000) = 1304

 $\theta = 3.4-72.7^{\circ}$ $\mu = 13.87 \text{ mm}^{-1}$ T = 100 KNeedle, yellow $0.13 \times 0.02 \times 0.02 \text{ mm}$

 $R_{\rm int} = 0.066$

 $h = -9 \rightarrow 5$

 $k = -13 \rightarrow 7$

 $l = -30 \rightarrow 31$

 $D_{\rm x} = 2.068 {\rm Mg} {\rm m}^{-3}$

Cu *Ka* radiation, $\lambda = 1.54184$ Å Cell parameters from 2416 reflections

4158 independent reflections

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

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

Crystal data

[Pt(C ₁₆ H ₁₈ N ₃)(NH ₃) ₂](NO ₃) ₂
$M_r = 668.97$
Monoclinic, $P2_1/c$
a = 7.6398 (3) Å
b = 10.8372 (11) Å
c = 25.982 (4) Å
$\beta = 92.478 \ (5)^{\circ}$
$V = 2149.1 (4) Å^3$
Z = 4

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

Refinement

Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	Only H-atom coordinates refined
$wR(F^2) = 0.155$	$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 7.5338P]$
S = 1.04	where $P = (F_0^2 + 2F_c^2)/3$
4158 reflections	$(\Delta/\sigma)_{\rm max} = 0.001$
304 parameters	$\Delta ho_{ m max} = 2.22 \ { m e} \ { m \AA}^{-3}$
444 restraints	$\Delta \rho_{\rm min} = -3.37 \text{ e } \text{\AA}^{-3}$

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.

x y z U_{w}^{+}/U_{π} Cl3 0.5794 (15) 1.0413 (10) 0.6474 (4) 0.024 (2) H13B 0.4831 1.1025 0.6463 0.028* Cl2 0.5652 (15) 1.0332 (10) 0.5942 (4) 0.024 (2) H12B 0.65618 1.0093 0.5689 0.029* H12B 0.6978 1.1162 0.5845 0.029* Cl1 0.8071 (15) 0.9424 (10) 0.5504 (5) 0.025 (2) H11B 0.9000 0.9621 0.6169 0.029* C9 0.7168 (13) 0.7372 (9) 0.5604 (4) 0.0187 (19) C8 0.7575 (13) 0.884 (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) 0.022 (2) H8 0.7111 0.9386 0.4135 0.031* C6 0.8915 (14) 0.780 (11) 0.4084 (4) 0.022 (2) C4B 0.818					TT J./TT	
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 $0.5652 (15)$ $1.0332 (10)$ $0.5942 (4)$ $0.024 (2)$ 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 0.94944 0.5561 $0.029*$ C9 $0.7168 (13)$ $0.7372 (9)$ $0.5064 (4)$ $0.0181 (18)$ C8A $0.7525 (13)$ $0.8684 (10)$ $0.4799 (4)$ $0.022 (2)$ H8 0.7111 0.9386 0.4965 $0.026*$ C7 $0.8178 (14)$ $0.789 (11)$ $0.4312 (4)$ $0.026 (2)$ H7 0.8093 0.9563 0.4135 $0.031*$ C6 $0.8915 (14)$ $0.789 (11)$ $0.4404 (4)$ $0.022 (2)$ H5 0.9377 0.5937 0.4131 $0.029*$ C4A $0.7001 (14)$ $0.5117 (10)$ $0.5402 (4)$ $0.020 (2)$ C4A $0.5601 (15)$ $0.3714 (11)$ $0.5923 (4)$ $0.022 (2)$ C4A $0.5021 (1)$ $0.5707 (4)$ $0.030*$ C2 $0.4806 (14)$ $0.6940 (10)$ $0.6216 (4)$ $0.024 (2)$ H4 $0.6941 (1)$ $0.5994 (1)$ $0.022 (2)$ C4A $0.5021 (1)$ $0.5995 (1)$ $0.5321 (1)$ $0.6904 (4)$		<i>x</i>	У	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$	
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C12 0.6562 (15) 1.0332 (10) 0.5942 (4) 0.029* H12A 0.5618 1.0093 0.5689 0.029* C11 0.8071 (15) 0.9424 (10) 0.5904 (5) 0.029* C11 0.8071 (15) 0.9424 (10) 0.5904 (5) 0.029* C11 0.8071 (15) 0.9424 (10) 0.5604 (4) 0.0181 (18) D.9000 0.9621 0.5604 (4) 0.0181 (18) 0.7372 (19) 0.5604 (4) 0.0122 (2) H8 0.7111 0.9386 0.4965 0.022* 0.775 (13) 0.8684 (10) 0.4799 (4) 0.022 (2) H8 0.7111 0.9386 0.4955 0.022* 0.775 (13) 0.8684 (10) 0.4312 (4) 0.026 (2) C7 0.8178 (14) 0.8798 (11) 0.4312 (4) 0.022 (2) 0.553 (4) 0.021 (2) C5 0.8907 (13) 0.6629 (11) 0.4084 (4) 0.022 (2) C4B 0.8181 (13) 0.6505 (10) 0.4788 (4) 0.022 (2) C4A 0.7001 (14) 0.5117 (10)	H13B	0.4831	1.1025	0.6463	0.028*	
H12A 0.5618 1.0093 0.5689 0.029* H12B 0.6978 1.1162 0.5845 0.029* H11A 0.8571 (15) 0.9424 (10) 0.5904 (5) 0.025 (2) H11A 0.8578 0.9494 0.5561 0.029* G2 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) H7 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) 0.4302 (4) 0.022 (2) C4B 0.8181 (13) 0.6505 (10) 0.4313 0.022 (2) C4A 0.7001 (14) 0.5117 (10) 0.5422 (4) 0.022 (2) C4A 0.6508 (14) 0.3219 0.5343 0.027* C3 0.5401 (15) 0.3714 (11) 0.5923 (4) 0.023 (2) </td <td>C12</td> <td>0.6562 (15)</td> <td>1.0332 (10)</td> <td>0.5942 (4)</td> <td>0.024 (2)</td> <td></td>	C12	0.6562 (15)	1.0332 (10)	0.5942 (4)	0.024 (2)	
H12B0.69781.11620.58450.029*C110.8071 (15)0.9424 (10)0.5904 (5)0.025 (2)H11A0.85780.94940.55610.029*C90.7168 (13)0.7372 (9)0.5604 (4)0.0187 (19)C8A0.7632 (13)0.7546 (9)0.5058 (4)0.0187 (19)C80.7575 (13)0.8684 (10)0.4799 (4)0.022 (2)H80.71110.93860.49650.026*C70.8178 (14)0.8798 (11)0.4132 (4)0.025 (2)H70.80930.95630.41350.031*C60.8915 (14)0.7780 (11)0.4084 (4)0.022 (2)H50.93070.59370.41310.029*C4B0.8181 (13)0.6505 (10)0.4788 (4)0.022 (2)C4A0.7001 (14)0.5117 (10)0.5402 (4)0.020 (2)C4A0.6508 (14)0.3901 (10)0.5529 (4)0.023 (2)C440.65400.32190.53430.027*C30.5401 (15)0.3714 (11)0.5923 (4)0.024 (2)C10.5925 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.282 (2)H17A0.41630.57990.70830.42*H17B0.23300.51240.71610.42*H17B0.23420.6	H12A	0.5618	1.0093	0.5689	0.029*	
C11 0.8071 (15) 0.9424 (10) 0.5904 (5) 0.025 (2) H11A 0.8578 0.9494 0.5561 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) 0.022 (2) H7 0.8093 0.9563 0.4135 0.031* C6 0.8915 (14) 0.7780 (11) 0.4084 (4) 0.022 (2) C4A 0.8181 (13) 0.6659 (10) 0.4788 (4) 0.022 (2) C4A 0.501 (10) 0.517 (10) 0.5402 (4) 0.022 (2) C4A 0.6504 (14) 0.391 (10) 0.5529 (4) 0.022 (2) C4A 0.6508 (14) 0.391 (10) 0.5259 (4) 0.022 (2) C4A 0.5032 0.2900 0.5998 <td< td=""><td>H12B</td><td>0.6978</td><td>1.1162</td><td>0.5845</td><td>0.029*</td><td></td></td<>	H12B	0.6978	1.1162	0.5845	0.029*	
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) 0.5058 (4) 0.0181 (18) C8A 0.7632 (13) 0.754 (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) 0.022 (2) H7 0.8093 0.9563 0.4135 0.031* C6 0.8915 (14) 0.7780 (11) 0.4302 (4) 0.022 (2) C5 0.8907 (13) 0.6629 (11) 0.4302 (4) 0.022 (2) C4B 0.8181 (13) 0.6505 (10) 0.4788 (4) 0.022 (2) C4A 0.5608 (14) 0.3901 (10) 0.5529 (4) 0.023 (2) C4A 0.6504 (14) 0.3901 (10) 0.5523 (4) 0.022 (2) C4A 0.5608 (14) 0.3901 (10) 0.5598 0.0	C11	0.8071 (15)	0.9424 (10)	0.5904 (5)	0.025 (2)	
H11B0.90000.96210.61690.029*C90.7168 (13)0.7372 (9)0.5604 (4)0.0181 (18)C8A0.7632 (13)0.7546 (9)0.5058 (4)0.0181 (18)C80.7575 (13)0.8684 (10)0.4799 (4)0.022 (2)H80.71110.93860.49650.026*C70.8178 (14)0.8798 (11)0.4312 (4)0.022 (2)H70.80930.95630.41350.031*C60.8915 (14)0.7780 (11)0.4084 (4)0.025 (2)C50.8907 (13)0.6629 (11)0.4302 (4)0.0224 (2)C4B0.8181 (13)0.6505 (10)0.4788 (4)0.022 (2)C4A0.7001 (14)0.5117 (10)0.5402 (4)0.020 (2)C440.6508 (14)0.3901 (10)0.5529 (4)0.022 (2)C440.6508 (14)0.3901 (10)0.5529 (4)0.022 (2)C440.50140.3901 (10)0.5529 (4)0.022 (2)C440.50320.29000.59980.0030*C50.4804 (15)0.3714 (11)0.5923 (4)0.022 (2)C140.5325 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (0)0.5707 (4)0.0180 (19)C170.3137 (15)0.51240.66850.042*H17A0.41630.57990.70830.042*H17A0.41630.57990.70830.030*C9A <t< td=""><td>H11A</td><td>0.8578</td><td>0.9494</td><td>0.5561</td><td>0.029*</td><td></td></t<>	H11A	0.8578	0.9494	0.5561	0.029*	
C9 $0.7168 (13)$ $0.7372 (9)$ $0.5604 (4)$ $0.0181 (18)$ C8A $0.7532 (13)$ $0.7546 (9)$ $0.5058 (4)$ $0.0127 (19)$ C8 $0.7575 (13)$ $0.8684 (10)$ $0.4799 (4)$ $0.022 (2)$ H8 0.7111 0.9386 0.4655 0.026^* C7 $0.8178 (14)$ $0.8798 (11)$ $0.4312 (4)$ $0.026 (2)$ H7 0.8093 0.9563 0.4135 $0.0121 (2)$ C5 $0.8915 (14)$ $0.7780 (11)$ $0.4084 (4)$ $0.022 (2)$ C5 $0.8907 (13)$ $0.6629 (11)$ $0.4302 (4)$ $0.024 (2)$ H5 0.9377 0.5937 0.4131 0.029^* C4B $0.8181 (13)$ $0.6505 (10)$ $0.788 (4)$ $0.020 (2)$ C4A $0.7001 (14)$ $0.5117 (10)$ $0.5402 (4)$ $0.020 (2)$ C4A $0.7001 (14)$ $0.5117 (10)$ $0.5402 (4)$ $0.022 (2)$ C4A $0.7001 (14)$ $0.5117 (10)$ $0.5529 (4)$ $0.023 (2)$ H4 0.6940 0.3219 0.5343 0.027^* C3 $0.5401 (15)$ $0.3714 (11)$ $0.5923 (4)$ $0.024 (2)$ C1 $0.5295 (13)$ $0.5870 (9)$ $0.6094 (4)$ $0.021 (2)$ C1 $0.5295 (13)$ $0.5870 (9)$ $0.6094 (4)$ $0.021 (2)$ C1 $0.5295 (13)$ $0.5170 (9)$ $0.022 *$ C3 $0.5466 (13)$ $0.6103 (9)$ $0.5707 (4)$ $0.1080 (19)$ C1 0.4228 0.6545 0.6425 0.304^* H17B 0.2340 <td>H11B</td> <td>0.9000</td> <td>0.9621</td> <td>0.6169</td> <td>0.029*</td> <td></td>	H11B	0.9000	0.9621	0.6169	0.029*	
C8A $0.7632 (13)$ $0.7546 (9)$ $0.5058 (4)$ $0.0187 (19)$ C8 $0.7575 (13)$ $0.8644 (10)$ $0.4799 (4)$ $0.022 (2)$ 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 $0.8915 (14)$ $0.7780 (11)$ $0.4084 (4)$ $0.022 (2)$ H5 0.9377 $0.6629 (11)$ $0.4302 (4)$ $0.022 (2)$ 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 $0.5401 (15)$ $0.3714 (11)$ $0.5923 (4)$ $0.022 (2)$ C4 0.5940 0.3219 0.5343 $0.027 *$ C3 $0.5401 (15)$ $0.3714 (11)$ $0.5923 (4)$ $0.022 (2)$ C4 0.5940 0.3219 0.5343 $0.027 *$ C3 $0.5401 (15)$ $0.3714 (11)$ $0.5923 (4)$ $0.024 (2)$ C1 $0.529 (13)$ $0.5870 (9)$ $0.6094 (4)$ $0.0181 (19)$ H1 0.4828 0.6545 0.6277 $0.022 *$ C9A $0.6466 (13)$ $0.6103 (9)$ $0.5707 (4)$ $0.0180 (19)$ C17 $0.3137 (15)$ $0.5425 (11)$ $0.6665 (4)$ $0.028 (2)$ H17A 0.4163	C9	0.7168 (13)	0.7372 (9)	0.5604 (4)	0.0181 (18)	
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) 0.022 (2) C5 0.8007 (13) 0.6502 (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 0.6508 (14) 0.5117 (10) 0.5523 (4) 0.023 (2) C4A 0.6508 (14) 0.3911 (10) 0.5523 (4) 0.022 (2) C4A 0.6508 (14) 0.3714 (11) 0.5923 (4) 0.025 (2) C3 0.5401 (15) 0.3714 (11) 0.5923 (4) 0.024 (2) C1 0.525 (13) 0.616 (4) 0.0181 (19) H1 0.4806 (14) 0.4697 0.6277 0.022*	C8A	0.7632 (13)	0.7546 (9)	0.5058 (4)	0.0187 (19)	
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) 0.022 (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) C4A 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) 0.5928 (4) 0.026 (2) H3 0.5032 0.2900 0.5998 0.030* C2 0.4806 (14) 0.6454 0.6277 0.022* C9A 0.6466 (13) 0.6103 (9) 0.5707 (4) 0.0180 (19)	C8	0.7575 (13)	0.8684 (10)	0.4799 (4)	0.022 (2)	
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 $0.029*$ $C4B$ $0.8181 (13)$ $0.6505 (10)$ $0.4788 (4)$ $0.022 (2)$ $C4A$ $0.7001 (14)$ $0.5117 (10)$ $0.5402 (4)$ $0.023 (2)$ $H4$ 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 $0.030*$ $C2$ $0.4806 (14)$ $0.4694 (10)$ $0.6216 (4)$ $0.0224 (2)$ $C1$ $0.5295 (13)$ $0.5870 (9)$ $0.6094 (4)$ $0.181 (19)$ $H1$ 0.4828 0.6545 0.6277 $0.022*$ $C9A$ $0.6466 (13)$ $0.613 (9)$ $0.5707 (4)$ $0.0180 (19)$ $C17$ $0.3137 (15)$ 0.5124 0.7683 $0.042*$ $H17A$ 0.4163 0.5799 0.7083 $0.042*$ $H17B$ 0.2330 0.5124 $0.6685 (0.022)$ $0.030*$ $H17B$ 0.2542 0.6685 $0.030*$ $H17A$ 0.4625 0.9330 0.6963 $0.030*$ $H17A$ 0.4625 0.9330 0.6963 $0.030*$ $H17A$ 0.4625 0.9330 0.6963 <td< td=""><td>H8</td><td>0.7111</td><td>0.9386</td><td>0.4965</td><td>0.026*</td><td></td></td<>	H8	0.7111	0.9386	0.4965	0.026*	
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^* H17B 0.2330 0.5124 0.6645 0.042^* N13 0.5114 (12) 0.9219 (8) 0.6653 (4) 0.0224 (19)N14 0.6632 0.9330 0.6963 0.030^* N9 0.7426 (10) 0.8136 (7) 0.5	C7	0.8178 (14)	0.8798 (11)	0.4312 (4)	0.026 (2)	
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 $0.8181 (13)$ $0.6505 (10)$ $0.4788 (4)$ $0.020 (2)$ 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 $0.5401 (15)$ $0.714 (11)$ $0.5923 (4)$ $0.024 (2)$ H3 0.5032 0.2900 0.5998 0.030^* C2 $0.4806 (14)$ $0.4694 (10)$ $0.616 (4)$ $0.024 (2)$ C1 $0.5295 (13)$ $0.5870 (9)$ $0.6094 (4)$ $0.0181 (19)$ H1 0.4828 0.6545 0.6277 0.022^* C9A $0.6466 (13)$ $0.613 (9)$ $0.5707 (4)$ $0.180 (19)$ 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^* H13D 0.4625 0.9330 0.6963 0.030^* N9 $0.7426 (10)$ $0.8136 (7)$ $0.5982 (3)$ $0.131 (15)$ N16 $0.9092 (13)$ $0.6683 (9)$ $0.6799 (4)$ $0.022 (1)$ N15 $0.9092 (13)$ $0.6683 (9)$ <	H7	0.8093	0.9563	0.4135	0.031*	
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 $0.5058(14)$ $0.3901(10)$ $0.552(4)$ $0.023(2)$ 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 $0.4466(13)$ $0.6103(9)$ $0.5707(4)$ $0.0180(19)$ 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 $0.030*$ H13D 0.4625 0.9330 0.6963 $0.030*$ H13D 0.4625 0.9330 0.6963 $0.030*$ H13D 0.4625 0.9330 0.6963 $0.030*$ N9 $0.7426(10)$ $0.8136(7)$ $0.5982(3)$ $0.0131(15)$ N16 $0.8018(12)$ $0.5329(9)$ $0.4987(4)$ $0.0224(19)$ N15 0.992	C6	0.8915 (14)	0.7780 (11)	0.4084 (4)	0.025 (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 0.4466 (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 0.5709 0.7083 0.042* H17C 0.2542 0.6042 0.6685 (4) 0.0247 (19)	C5	0.8907 (13)	0.6629 (11)	0.4302 (4)	0.024 (2)	
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 0.6103 (9) 0.5707 (4) 0.0180 (19) C17 0.3137 (15) 0.5425 (11) 0.6006 (4) 0.028 (2) H17A 0.4163 0.5799 0.7083 0.042* H17D 0.2330 0.5124 0.7161 0.042* H17C 0.2542 0.6042 0.6685 0.042* N13 0.5114 (12) 0.9219 (8) 0.66635 (4) 0.0227 (19)	Н5	0.9377	0.5937	0.4131	0.029*	
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 $0.0247(19)$ H17C 0.2542 0.6042 0.6685 $0.042*$ N13 $0.5114(12)$ $0.9219(8)$ $0.653(4)$ $0.0247(19)$ 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 $0.9992(13)$ $0.6683(9)$ $0.6799(4)$ $0.0224(19)$ N15 $0.9922(13)$ 0.6636 0.6494 $0.042*$ H15B 0.9632 0.6636 0.6494 $0.042*$ H15A 0.9869 0.6955 0.7049 $0.042*$ H15B </td <td>C4B</td> <td>0.8181 (13)</td> <td>0.6505 (10)</td> <td>0.4788 (4)</td> <td>0.022 (2)</td> <td></td>	C4B	0.8181 (13)	0.6505 (10)	0.4788 (4)	0.022 (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 $0.42*$ 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)H13D 0.4625 0.9330 0.6963 $0.30*$ 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 $0.042*$ H15B 0.9632 0.6636 0.6494 $0.042*$ H15B 0.9632 0.6636 0.6494 $0.042*$ <	C4A	0.7001 (14)	0.5117 (10)	0.5402 (4)	0.020 (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 0.30^* 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 $0.5114 (12)$ $0.9219 (8)$ $0.6653 (4)$ $0.0247 (19)$ H13D 0.4625 0.9330 0.6963 0.030^* N9 $0.7426 (10)$ $0.8136 (7)$ $0.5982 (3)$ $0.0131 (15)$ N10 $0.8018 (12)$ $0.5329 (9)$ $0.497 (4)$ $0.0224 (19)$ N15 $0.9092 (13)$ $0.6633 (9)$ $0.6799 (4)$ $0.0228 (2)$ 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 0.6614 0.6801 0.7557 0.045^* H14B 0.5588 0.7965 0.7680 0.045^* <td>C4</td> <td>0.6508 (14)</td> <td>0.3901 (10)</td> <td>0.5529 (4)</td> <td>0.023 (2)</td> <td></td>	C4	0.6508 (14)	0.3901 (10)	0.5529 (4)	0.023 (2)	
C30.5401 (15)0.3714 (11)0.5923 (4)0.025 (2)H30.50320.29000.59980.030*C20.4806 (14)0.4694 (10)0.6216 (4)0.024 (2)C10.5295 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*H13D0.46250.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.6636 (0.64940.042*H15C0.86930.59230.68850.042*H15A0.8603 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	H4	0.6940	0.3219	0.5343	0.027*	
H30.50320.29000.59980.030*C20.4806 (14)0.4694 (10)0.6216 (4)0.024 (2)C10.5295 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14B0.55880.79650.75690.045*H14B0.55880.79650.75690.045*	C3	0.5401 (15)	0.3714 (11)	0.5923 (4)	0.025 (2)	
C20.4806 (14)0.4694 (10)0.6216 (4)0.024 (2)C10.5295 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.0228 (2)H15A0.9690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.66140.68010.75570.045*N14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*H14C0.75120.79880.76800.045*	H3	0.5032	0.2900	0.5998	0.030*	
C10.5295 (13)0.5870 (9)0.6094 (4)0.0181 (19)H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7458 (3)0.030 (2)H14A0.66140.68010.75570.045*H14E0.55880.79650.76800.045*	C2	0.4806 (14)	0.4694 (10)	0.6216 (4)	0.024 (2)	
H10.48280.65450.62770.022*C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	C1	0.5295 (13)	0.5870 (9)	0.6094 (4)	0.0181 (19)	
C9A0.6466 (13)0.6103 (9)0.5707 (4)0.0180 (19)C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.30*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76690.045*	H1	0.4828	0.6545	0.6277	0.022*	
C170.3137 (15)0.5425 (11)0.6906 (4)0.028 (2)H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	C9A	0.6466 (13)	0.6103 (9)	0.5707 (4)	0.0180 (19)	
H17A0.41630.57990.70830.042*H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	C17	0.3137 (15)	0.5425 (11)	0.6906 (4)	0.028 (2)	
H17B0.23300.51240.71610.042*H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	H17A	0.4163	0.5799	0.7083	0.042*	
H17C0.25420.60420.66850.042*N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*H14C0.75120.79880.76800.045*	H17B	0.2330	0.5124	0.7161	0.042*	
N130.5114 (12)0.9219 (8)0.6653 (4)0.0247 (19)H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	H17C	0.2542	0.6042	0.6685	0.042*	
H13C0.42580.89520.64250.030*H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	N13	0.5114 (12)	0.9219 (8)	0.6653 (4)	0.0247 (19)	
H13D0.46250.93300.69630.030*N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	H13C	0.4258	0.8952	0.6425	0.030*	
N90.7426 (10)0.8136 (7)0.5982 (3)0.0131 (15)N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	H13D	0.4625	0.9330	0.6963	0.030*	
N100.8018 (12)0.5329 (9)0.4987 (4)0.0224 (19)N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.76800.045*	N9	0.7426 (10)	0.8136 (7)	0.5982 (3)	0.0131 (15)	
N150.9092 (13)0.6683 (9)0.6799 (4)0.028 (2)H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	N10	0.8018 (12)	0.5329 (9)	0.4987 (4)	0.0224 (19)	
H15A0.98690.69550.70490.042*H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	N15	0.9092 (13)	0.6683 (9)	0.6799 (4)	0.028 (2)	
H15B0.96320.66360.64940.042*H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	H15A	0.9869	0.6955	0.7049	0.042*	
H15C0.86930.59230.68850.042*N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	H15B	0.9632	0.6636	0.6494	0.042*	
N140.6630 (14)0.7624 (9)0.7488 (3)0.030 (2)H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	H15C	0.8693	0.5923	0.6885	0.042*	
H14A0.66140.68010.75570.045*H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	N14	0.6630 (14)	0.7624 (9)	0.7488 (3)	0.030 (2)	
H14B0.55880.79650.75690.045*H14C0.75120.79880.76800.045*	H14A	0.6614	0.6801	0.7557	0.045*	
H14C 0.7512 0.7988 0.7680 0.045*	H14B	0.5588	0.7965	0.7569	0.045*	
	H14C	0.7512	0.7988	0.7680	0.045*	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

0 1917 (13)	0 8899 (10)	0 7529 (4)	0.031(2)	
1.1839 (13)	0.7603 (9)	0.5780 (4)	0.0285(19)	
0.3694 (10)	0.4397 (7)	0.6591 (3)	0.0281 (17)	
0.2424 (13)	0.7816 (9)	0.7465 (4)	0.046 (2)	
0.0363 (12)	0.9147 (10)	0.7567 (4)	0.052 (3)	
0.3072 (12)	0.9761 (9)	0.7549 (4)	0.039 (2)	
1.1896 (10)	0.8149 (7)	0.6210 (3)	0.0280 (17)	
1.1044 (11)	0.6585 (7)	0.5742 (3)	0.0304 (18)	
1.2554 (14)	0.8075 (8)	0.5413 (4)	0.047 (2)	
0.9803 (4)	0.7921 (3)	0.34724 (11)	0.0360 (7)	
0.70226 (6)	0.78889 (4)	0.67275 (2)	0.02123 (16)	
0.816 (17)	0.483 (12)	0.481 (5)	0.025*	
	$\begin{array}{c} 0.1917\ (13)\\ 1.1839\ (13)\\ 0.3694\ (10)\\ 0.2424\ (13)\\ 0.0363\ (12)\\ 0.3072\ (12)\\ 1.1896\ (10)\\ 1.1044\ (11)\\ 1.2554\ (14)\\ 0.9803\ (4)\\ 0.70226\ (6)\\ 0.816\ (17)\\ \end{array}$	$\begin{array}{cccccc} 0.1917(13) & 0.8899(10) \\ 1.1839(13) & 0.7603(9) \\ 0.3694(10) & 0.4397(7) \\ 0.2424(13) & 0.7816(9) \\ 0.0363(12) & 0.9147(10) \\ 0.3072(12) & 0.9761(9) \\ 1.1896(10) & 0.8149(7) \\ 1.1044(11) & 0.6585(7) \\ 1.2554(14) & 0.8075(8) \\ 0.9803(4) & 0.7921(3) \\ 0.70226(6) & 0.78889(4) \\ 0.816(17) & 0.483(12) \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Atomic displacement parameters $(Å^2)$

	x 711	T 7))	T 72.2	x 12	x r12	x 7)2
	U	U ²²	U^{ss}	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)
01	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)
019A	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)
C16	0.0408 (15)	0.0412 (17)	0.0271 (14)	-0.0127 (15)	0.0124 (12)	-0.0027 (13)

						data reports
Pt	0.0231 (2)	0.0156 (2)	0.0255 (3)	0.0002 (2)	0.00693 (17)	0.0003 (2)
Geome	tric parameters (Å,	. ?)				
C13—I	H13A	0.9900		С3—Н3	0.	9500
C13—I	H13B	0.9900		С3—С2	1.	393 (16)
C13—0	C12	1.527 (14	-)	C2—C1	1.	370 (15)
C13—1	N13	1.477 (13		C2—O1	1.	359 (13)
C12—I	H12A	0.9900		C1—H1	0.	9500
C12—I	H12B	0.9900		C1—C9A	1.	398 (13)
C12—0	C11	1.522 (14	•)	C17—H17A	0.	9800
C11—I	H11A	0.9900		C17—H17B	0.	9800
C11—I	H11B	0.9900		C17—H17C	0.	9800
C11—1	N9	1.497 (12	2)	C17—O1	1.	457 (13)
С9—С	8A	1.489 (14	.)	N13—H13C	0.	9100
С9—С	9A	1.504 (14	-)	N13—H13D	0.	9100
C9—N	9	1.293 (13	5)	N13—Pt	2.	053 (9)
C8A—	C8	1.404 (15	5)	N9—Pt	1.	993 (8)
C8A—	C4B	1.402 (14	-)	N10—H10	0.	72 (12)
С8—Н	8	0.9500	, ,	N15—H15A	0.	9100
C8—C	7	1.371 (14	-)	N15—H15B	0.	9100
С7—Н	7	0.9500	,	N15—H15C	0.	9100
С7—С	6	1.384 (16	5)	N15—Pt	2.	053 (10)
С6—С	5	1.371 (16	5)	N14—H14A	0.	9100
С6—С	16	1.760 (11)	N14—H14B	0.	9100
С5—Н	5	0.9500	/	N14—H14C	0.	9100
С5—С	4B	1.407 (14	-)	N14—Pt	2.	033 (9)
C4B—	N10	1.383 (14	-) -)	N18—018C	1.	249 (13)
C4A—	C4	1.414 (14	-) -)	N18—018B	1.	225 (13)
C4A—	C9A	1.402 (14	-) -)	N18—018A	1.	284 (13)
C4A—	N10	1.374 (14	-) -)	N19-019A	1.	262 (12)
С4—Н	4	0.9500	/	N19—019B	1.	261 (13)
C4—C	3	1.370 (15	i)	N19—019C	1.	231 (13)
H13A-	C13H13B	107.8		O1—C2—C1	12	24.8 (10)
C12—0	C13—H13A	109.0		C2—C1—H1	11	19.2
C12—0	C13—H13B	109.0		C2-C1-C9A	12	21.6 (10)
N13—	С13—Н13А	109.0		C9A—C1—H1	11	19.2
N13—	С13—Н13В	109.0		C4A—C9A—C9	11	18.8 (9)
N13—	C13—C12	112.9 (9)		C1—C9A—C9	12	22.4 (9)
C13—0	C12—H12A	108.6		C1—C9A—C4A	11	18.8 (9)
C13—0	C12—H12B	108.6		H17A—C17—H17B	3 10	09.5
H12A-	C12H12B	107.6		H17A—C17—H17C	2 10	09.5
C11—0	C12—C13	114.7 (9)		H17B—C17—H17C	10	09.5
C11—0	C12—H12A	108.6		O1—C17—H17A	10	09.5
C11—0	C12—H12B	108.6		O1—C17—H17B	10	09.5
C12—0	C11—H11A	109.7		O1—C17—H17C	10	09.5
C12—0	С11—Н11В	109.7		C13—N13—H13C	10	09.0

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)
С8А—С8—Н8	119.5	C4A—N10—H10	119 (10)
C7—C8—C8A	121.1 (10)	H15A—N15—H15B	109.5
С7—С8—Н8	119.5	H15A—N15—H15C	109.5
С8—С7—Н7	120.5	H15B—N15—H15C	109.5
C8—C7—C6	118.9 (11)	Pt—N15—H15A	109.5
С6—С7—Н7	120.5	Pt—N15—H15B	109.5
C7—C6—C16	119.9 (9)	Pt—N15—H15C	109.5
C5—C6—C7	122.5 (10)	H14A—N14—H14B	109.5
C5—C6—C16	117.5 (9)	H14A—N14—H14C	109.5
С6—С5—Н5	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)
С4—С3—Н3	119.3	N9—Pt—N15	91.3 (4)
C4—C3—C2	121.5 (10)	N9—Pt—N14	179.5 (4)
С2—С3—Н3	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, °)

D—H···A	D—H	H···A	D····A	D—H···A
N10—H10…O19B ⁱ	0.72 (12)	2.20 (12)	2.919 (12)	172 (14)
N13—H13 <i>C</i> ···O19 <i>A</i> 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 ⁱⁱⁱⁱ	0.91	2.24	3.113 (14)	160
N14—H14 <i>B</i> ····O18 <i>C</i>	0.91	2.43	3.218 (15)	146
N14—H14 <i>C</i> ···O18 <i>B</i> ^{iv}	0.91	2.54	3.294 (15)	140
N14—H14 C ···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···O19 <i>C</i> ⁱ	0.95	2.46	3.354 (14)	157	
C7—H7…O19 <i>A</i> ^{vi}	0.95	2.64	3.576 (14)	170	
C11—H11 <i>B</i> ····Cl6 ^{vi}	0.99	2.95	3.649 (12)	128	
C17—H17A…O18A ⁱⁱⁱ	0.98	2.54	3.250 (15)	129	
C17—H17 <i>B</i> ····O18 <i>B</i> ^{vii}	0.98	2.45	3.356 (15)	154	
С17—Н17С…О19А ^{іі}	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.