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# (Cyclobutane-1,1-dicarboxylato-$\kappa^2O,O'$)-(1,10-phenanthroline-$\kappa^2N,N'$)-platinum(II) dihydrate

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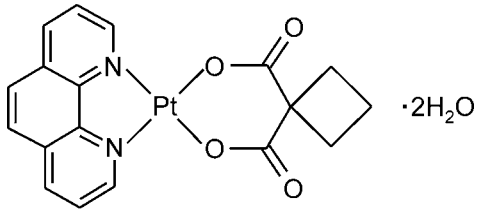
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.021; $wR$ factor = 0.058; data-to-parameter ratio = 11.6.

The title compound, $[Pt(C_6H_6O_4)(C_{12}H_8N_2)]\cdot 2H_2O$, which crystallizes as two independent formula units, has the metal atom in a square-planar geometry defined by two O atoms of the chelating cyclobutane-1,1-dicarboxylate dianion and two N atoms of the chelating 1,10-phenanthroline molecule (r.m.s. deviations of the $PtO_2N_2$ units = 0.026 and 0.026 Å). Adjacent complex and water molecules are connected through intermolecular O—H···O hydrogen bonds and C—H···O, C···O [shortest C···O distance = 3.140 (5) Å], $\pi$–$\pi$ [shortest C···C distances = 3.234 (6) and 3.347 (6) Å] and Pt···$\pi$ [shortest Pt···C distance = 3.358 (4) Å] interactions into a three-dimensional network.

## Related literature

For platinum(II) cyclobutane-1,1-dicarboxylate complexes of other bidentate heterocyclic *N*-donor ligands, see: Ferreira *et al.* (1997); Yoo *et al.* (1999); Tu *et al.* (2003, 2004).




## Experimental

### Crystal data

$[Pt(C_6H_6O_4)(C_{12}H_8N_2)]\cdot 2H_2O$
$M_r$ = 553.43
Triclinic, $P\overline{1}$
$a$ = 10.93439 (14) Å
$b$ = 11.83205 (18) Å
$c$ = 13.51039 (19) Å
$\alpha$ = 84.7158 (12)°
$\beta$ = 84.3918 (11)°
$\gamma$ = 85.6240 (11)°
$V$ = 1728.17 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 8.16 mm$^{-1}$
$T$ = 100 K
0.30 × 0.30 × 0.25 mm

### Data collection

Agilent Xcalibur Sapphire2 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.193, $T_{max}$ = 0.235
13766 measured reflections
6042 independent reflections
5691 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.058
$S$ = 1.12
6042 reflections
519 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.89 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5*W*···O6 | 0.84 | 1.97 | 2.802 (5) | 170 |
| O6—H6*W*···O3 | 0.83 | 2.03 | 2.842 (4) | 165 |
| O7—H7*W*···O3*A* | 0.83 | 1.93 | 2.753 (4) | 169 |
| O8—H8*V*···O7 | 0.85 | 1.95 | 2.806 (5) | 175 |
| O5—H5*V*···O8$^{i}$ | 0.85 | 1.98 | 2.821 (5) | 169 |
| O6—H6*V*···O4$^{ii}$ | 0.84 | 2.00 | 2.839 (4) | 173 |
| O7—H7*V*···O4*A*$^{iii}$ | 0.83 | 2.00 | 2.828 (4) | 176 |
| O8—H8*W*···O1$^{iv}$ | 0.84 | 2.43 | 3.125 (4) | 142 |
| O8—H8*W*···O3$^{iv}$ | 0.84 | 2.17 | 2.971 (4) | 160 |
| C7*A*—H7*AA*···O3$^{iv}$ | 0.95 | 2.55 | 3.376 (5) | 146 |
| C7—H7*A*···O7$^{iv}$ | 0.95 | 2.49 | 3.145 (5) | 126 |
| C8—H8*A*···O5$^{v}$ | 0.95 | 2.59 | 3.259 (6) | 128 |
| C9—H9*A*···O6$^{v}$ | 0.95 | 2.51 | 3.436 (6) | 165 |
| C14*A*—H14*A*···O8$^{vi}$ | 0.95 | 2.35 | 3.230 (6) | 154 |
| C14—H14*B*···O5$^{vii}$ | 0.95 | 2.36 | 3.309 (6) | 174 |
| C18*A*—H18*A*···O4*A*$^{v}$ | 0.95 | 2.38 | 3.196 (5) | 144 |
| C18—H18*B*···O4$^{v}$ | 0.95 | 2.55 | 3.151 (5) | 121 |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5330).

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# supporting information

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# (Cyclobutane-1,1-dicarboxylato-$\kappa^2O,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)platinum(II) dihydrate

**Pavel Štarha and Zdeněk Trávníček**

## S1. Comment

The asymmetric unit of the title complex, [Pt(cbdc)(phen)].2$H_2O$, (I), (Figure 1), contains two independent molecules of the complex and four water molecules of crystallization. The $Pt^{II}$ atom is four-coordinated by two oxygen (cyclobutane-1,1-dicarboxylate dianion; cbdc) and two nitrogen (1,10-phenathroline; phen) atoms. The geometry is distorted square-planar with the N–Pt–O angles equalled to 92.64 (12)° and 93.57 (12)° for Pt1-molecule, and 93.18 (11)° and 93.25 (12)° for Pt2-molecule. The planes fitted through the $Pt1O_2N_2$ (r.m.s. deviation 0.026 Å) and $Pt2O_2N_2$ (r.m.s. deviation 0.026 Å) units form the dihedral angle of 61.42 (8)°, while the dihedral angle formed by both phen molecules is 63.34 (4)°. This corresponds with nearly coplanar orientation of the phen molecule and $PtO_2N_2$ unit (a dihedral angle of 3.57 (7)° for Pt1-molecule, and 2.58 (8)° for Pt2-molecule). The crystal structure contains O—H···O hydrogen bonds and C—H···O, C···O, $\pi$–$\pi$ (the shortest C···C distances equal 3.234 (6) Å for C8···C16$^{viii}$ and 3.347 (6) Å for C8A···C16A$^{vi}$; symmetry codes: viii) –x+1, –y, –z; vi) –x, –y+1, –z+1) and Pt···$\pi$ (the shortest Pt···C distance equals 3.358 (4) Å for Pt1···C10$^{viii}$) types of the non-covalent contacts, which connect the molecules into a three-dimensional architecture (Figure 2, Table 1). The Pt1···Pt2, Pt1···Pt1$^{viii}$ and Pt2···Pt2$^{vi}$ distances are 7.8526 (2) Å, 5.2788 (2) Å, and 4.9992 (2) Å, respectively.

## S2. Experimental

Warm (60 °C) distilled-water solutions of [Pt(cbdc)$(dmso)_2$] (0.25 mmol) and 1,10-phenanthroline (0.25 mmol) were mixed together and stirred at 60 °C for 24 h. After that, the mixture was filtered and left to crystallize. The crystalline product, which formed in two weeks, was filtered off and washed with distilled water and methanol. Several crystals were collected for a single-crystal X-ray analysis. CH&N analysis calculated for $C_{18}H_{18}N_2O_6Pt_1$: C 39.1, H 3.3, N 5.1%; found: C 39.2, H 3.3, N 5.3%. Elemental analysis (CH&N) was performed on a Thermo Scientific Flash 2000 CHNO-S Analyzer.

## S3. Refinement

Non-hydrogen atoms were refined anisotropically and hydrogen atoms were located in difference maps and refined using the riding model with C—H = 0.95 (CH), C—H = 0.99 ($CH_2$) Å, with $U_{iso}$(H) = 1.2$U_{eq}$(CH, $CH_2$). The maximum and minimum residual electron density peaks of 1.27 and -0.89 e Å$^{-3}$ were located 0.94 Å, and 0.78 Å from the Pt1, and Pt2 atoms, respectively.

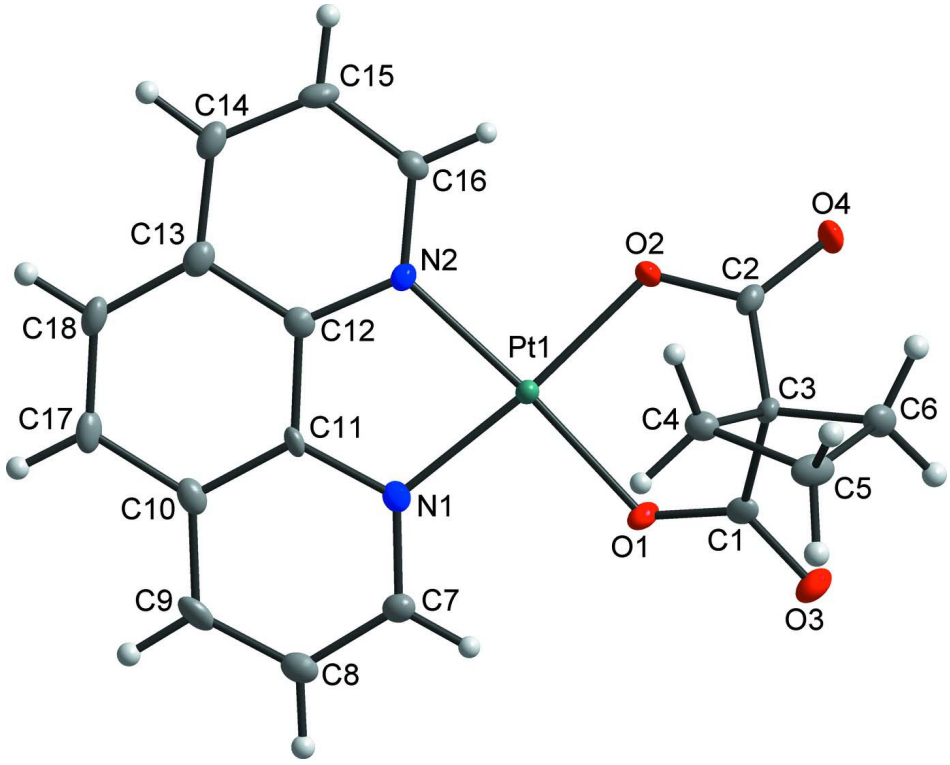


**Figure 1**

The molecular structure (one of two independent molecules within the asymmetric unit) of the title complex with the non-hydrogen atoms depicted as thermal ellipsoids at the 50% probability level.

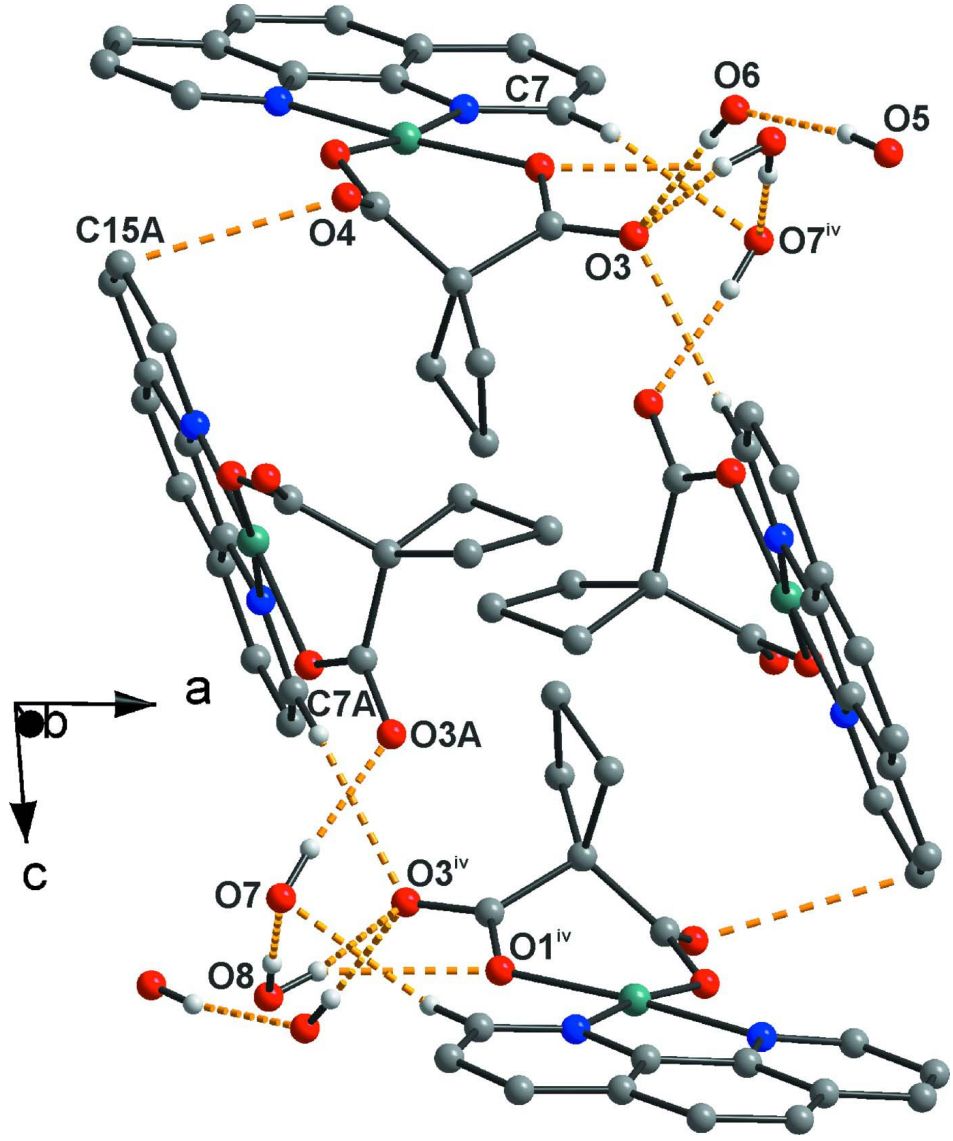


**Figure 2**

Part of the crystal structure of (I) showing the selected O5—H5W···O6, O6—H6W···O3, O7—H7W···O3A, O8—H8V···O7, O8—H8W···O1$^{iv}$ and O8—H8W···O3$^{iv}$ hydrogen bonds, and C7—H7A···O7$^{iv}$ (D—H, H···A, D···A (Å)and <DHA (°): 0.95, 2.49, 3.145 (6), 126), C7A—H7AA···O3$^{iv}$ (0.95, 2.55, 3.376 (6), 146) and C15A···O4 (D···A (Å): 3.140 (5)) non-covalent contacts (dashed orange lines); symmetry code: iv) –x+1, –y+1, –z+1; (see Table 1 for the parameters of O—H···O hydrogen bonds).

**(Cyclobutane-1,1-dicarboxylato-$\kappa^2O,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)platinum(II) dihydrate**

*Crystal data*

$[Pt(C_6H_6O_4)(C_{12}H_8N_2)]\cdot 2H_2O$
$M_r$ = 553.43
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 10.93439 (14) Å
$b$ = 11.83205 (18) Å
$c$ = 13.51039 (19) Å
$\alpha$ = 84.7158 (12)°
$\beta$ = 84.3918 (11)°
$\gamma$ = 85.6240 (11)°
$V$ = 1728.17 (4) Å$^3$
$Z$ = 4

$F(000) = 1064$
$D_x = 2.127$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17004 reflections
$\theta = 3.0–31.9°$
$\mu = 8.16$ mm$^{-1}$
$T = 100$ K
Prism, yellow
0.30 × 0.30 × 0.25 mm

*Data collection*

Agilent Xcalibur Sapphire2 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 8.3611 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.193$, $T_{max} = 0.235$
13766 measured reflections
6042 independent reflections
5691 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.058$
$S = 1.12$
6042 reflections
519 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 3.750P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.27$ e Å$^{-3}$
$\Delta\rho_{min} = -0.89$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1A | 0.1984 (3) | 0.7390 (2) | 0.5535 (2) | 0.0159 (6) |
| N1A | 0.1813 (3) | 0.4983 (3) | 0.5337 (2) | 0.0129 (7) |
| C1A | 0.2499 (4) | 0.8338 (4) | 0.5299 (3) | 0.0148 (9) |
| Pt1 | 0.453703 (13) | 0.146225 (12) | 0.137337 (10) | 0.00981 (6) |
| O1 | 0.6022 (2) | 0.2325 (2) | 0.1494 (2) | 0.0142 (6) |
| N1 | 0.5504 (3) | −0.0034 (3) | 0.1351 (2) | 0.0117 (7) |
| C1 | 0.5956 (4) | 0.3279 (3) | 0.1894 (3) | 0.0119 (8) |
| Pt2 | 0.156255 (13) | 0.642655 (12) | 0.448083 (10) | 0.01040 (6) |
| O2A | 0.1157 (3) | 0.7813 (2) | 0.3578 (2) | 0.0146 (6) |
| N2A | 0.1119 (3) | 0.5367 (3) | 0.3526 (2) | 0.0139 (7) |

| | | | | |
|---|---|---|---|---|
| C2A | 0.1688 (4) | 0.8749 (3) | 0.3638 (3) | 0.0124 (8) |
| N2 | 0.3162 (3) | 0.0506 (3) | 0.1192 (2) | 0.0117 (7) |
| O2 | 0.3455 (2) | 0.2901 (2) | 0.1274 (2) | 0.0144 (6) |
| C2 | 0.3757 (4) | 0.3818 (4) | 0.1618 (3) | 0.0138 (8) |
| C3A | 0.2857 (4) | 0.8653 (4) | 0.4187 (3) | 0.0150 (9) |
| O3A | 0.2689 (3) | 0.8974 (3) | 0.5925 (2) | 0.0224 (7) |
| O3 | 0.6886 (3) | 0.3818 (3) | 0.1888 (2) | 0.0184 (6) |
| C3 | 0.4711 (4) | 0.3702 (3) | 0.2382 (3) | 0.0119 (8) |
| O4A | 0.1305 (3) | 0.9664 (2) | 0.3257 (2) | 0.0194 (6) |
| C4A | 0.3951 (4) | 0.7854 (4) | 0.3772 (3) | 0.0160 (9) |
| H4AA | 0.4094 | 0.7139 | 0.4198 | 0.019* |
| H4AB | 0.3915 | 0.7702 | 0.3067 | 0.019* |
| O4 | 0.3279 (3) | 0.4755 (2) | 0.1359 (2) | 0.0197 (7) |
| C4 | 0.4412 (4) | 0.2950 (4) | 0.3374 (3) | 0.0144 (8) |
| H4A | 0.3528 | 0.2818 | 0.3524 | 0.017* |
| H4B | 0.4929 | 0.2227 | 0.3433 | 0.017* |
| C5A | 0.4822 (4) | 0.8787 (4) | 0.3913 (3) | 0.0199 (9) |
| H5AA | 0.5246 | 0.8649 | 0.4532 | 0.024* |
| H5AB | 0.5415 | 0.8956 | 0.3326 | 0.024* |
| C5 | 0.4845 (4) | 0.3897 (4) | 0.3947 (3) | 0.0194 (9) |
| H5A | 0.5692 | 0.3745 | 0.4149 | 0.023* |
| H5B | 0.4262 | 0.4110 | 0.4518 | 0.023* |
| O5 | 0.9600 (3) | 0.7036 (3) | 0.0445 (3) | 0.0242 (7) |
| C6A | 0.3696 (4) | 0.9654 (4) | 0.3991 (3) | 0.0189 (9) |
| H6AA | 0.3674 | 1.0129 | 0.4560 | 0.023* |
| H6AB | 0.3572 | 1.0130 | 0.3363 | 0.023* |
| C6 | 0.4756 (4) | 0.4727 (4) | 0.2997 (3) | 0.0184 (9) |
| H6A | 0.3996 | 0.5238 | 0.3011 | 0.022* |
| H6B | 0.5495 | 0.5162 | 0.2815 | 0.022* |
| O6 | 0.8025 (3) | 0.5297 (3) | 0.0351 (2) | 0.0258 (7) |
| C7A | 0.2141 (4) | 0.4841 (4) | 0.6263 (3) | 0.0165 (9) |
| H7AA | 0.2312 | 0.5486 | 0.6584 | 0.020* |
| C7 | 0.6712 (4) | −0.0248 (4) | 0.1398 (3) | 0.0146 (8) |
| H7A | 0.7204 | 0.0350 | 0.1505 | 0.017* |
| O7 | 0.1062 (3) | 0.9814 (3) | 0.7410 (2) | 0.0262 (8) |
| C8 | 0.7264 (4) | −0.1337 (4) | 0.1292 (3) | 0.0167 (9) |
| H8A | 0.8128 | −0.1470 | 0.1325 | 0.020* |
| C8A | 0.2239 (4) | 0.3760 (4) | 0.6776 (3) | 0.0224 (10) |
| H8AA | 0.2466 | 0.3679 | 0.7441 | 0.027* |
| O8 | 0.1100 (3) | 0.7860 (3) | 0.8755 (3) | 0.0251 (7) |
| C9A | 0.2008 (4) | 0.2815 (4) | 0.6324 (3) | 0.0217 (10) |
| H9AA | 0.2082 | 0.2083 | 0.6675 | 0.026* |
| C9 | 0.6574 (4) | −0.2223 (4) | 0.1142 (3) | 0.0167 (9) |
| H9A | 0.6957 | −0.2960 | 0.1056 | 0.020* |
| C10A | 0.1663 (4) | 0.2928 (4) | 0.5345 (3) | 0.0175 (9) |
| C10 | 0.5291 (4) | −0.2017 (3) | 0.1117 (3) | 0.0140 (8) |
| C11A | 0.1572 (3) | 0.4046 (3) | 0.4885 (3) | 0.0123 (8) |
| C11 | 0.4803 (4) | −0.0907 (3) | 0.1219 (3) | 0.0099 (8) |

| | | | | |
|---|---|---|---|---|
| C12A | 0.1200 (3) | 0.4261 (3) | 0.3902 (3) | 0.0122 (8) |
| C12 | 0.3531 (4) | −0.0603 (3) | 0.1137 (3) | 0.0122 (8) |
| C13A | 0.0898 (4) | 0.3367 (4) | 0.3380 (3) | 0.0172 (9) |
| C13 | 0.2739 (4) | −0.1442 (4) | 0.0995 (3) | 0.0151 (9) |
| C14A | 0.0511 (4) | 0.3660 (4) | 0.2424 (3) | 0.0200 (9) |
| H14A | 0.0291 | 0.3086 | 0.2040 | 0.024* |
| C14 | 0.1496 (4) | −0.1059 (4) | 0.0891 (3) | 0.0161 (9) |
| H14B | 0.0908 | −0.1585 | 0.0805 | 0.019* |
| C15A | 0.0451 (4) | 0.4774 (4) | 0.2046 (3) | 0.0202 (10) |
| H15A | 0.0196 | 0.4972 | 0.1397 | 0.024* |
| C15 | 0.1151 (4) | 0.0079 (4) | 0.0915 (3) | 0.0165 (9) |
| H15B | 0.0325 | 0.0345 | 0.0820 | 0.020* |
| C16A | 0.0763 (4) | 0.5623 (4) | 0.2614 (3) | 0.0158 (9) |
| H16A | 0.0719 | 0.6393 | 0.2344 | 0.019* |
| C16 | 0.1994 (4) | 0.0843 (4) | 0.1076 (3) | 0.0131 (8) |
| H16B | 0.1732 | 0.1625 | 0.1104 | 0.016* |
| C17A | 0.1382 (4) | 0.2005 (4) | 0.4768 (3) | 0.0197 (9) |
| H17A | 0.1466 | 0.1240 | 0.5048 | 0.024* |
| C17 | 0.4475 (4) | −0.2880 (4) | 0.1002 (3) | 0.0156 (9) |
| H17B | 0.4782 | −0.3650 | 0.0969 | 0.019* |
| C18A | 0.1011 (4) | 0.2228 (4) | 0.3857 (3) | 0.0210 (10) |
| H18A | 0.0812 | 0.1615 | 0.3509 | 0.025* |
| C18 | 0.3240 (4) | −0.2579 (4) | 0.0939 (3) | 0.0169 (9) |
| H18B | 0.2706 | −0.3152 | 0.0855 | 0.020* |
| H5V | 0.996 (5) | 0.731 (5) | −0.010 (3) | 0.05 (2)* |
| H5W | 0.919 (4) | 0.649 (3) | 0.036 (4) | 0.028 (14)* |
| H6V | 0.759 (5) | 0.526 (6) | −0.012 (3) | 0.06 (2)* |
| H6W | 0.776 (4) | 0.477 (3) | 0.074 (3) | 0.024 (14)* |
| H7V | 0.038 (3) | 0.996 (5) | 0.718 (4) | 0.038 (16)* |
| H7W | 0.151 (4) | 0.948 (4) | 0.698 (3) | 0.030 (15)* |
| H8V | 0.109 (6) | 0.843 (4) | 0.832 (4) | 0.05 (2)* |
| H8W | 0.177 (3) | 0.753 (5) | 0.856 (4) | 0.042 (17)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1A | 0.0166 (15) | 0.0163 (16) | 0.0153 (14) | −0.0036 (12) | −0.0017 (11) | −0.0012 (12) |
| N1A | 0.0088 (16) | 0.0150 (19) | 0.0144 (17) | −0.0021 (13) | −0.0003 (13) | 0.0013 (14) |
| C1A | 0.013 (2) | 0.014 (2) | 0.017 (2) | 0.0004 (16) | −0.0020 (16) | −0.0025 (17) |
| Pt1 | 0.00974 (9) | 0.00862 (10) | 0.01139 (9) | −0.00119 (6) | −0.00273 (6) | −0.00017 (6) |
| O1 | 0.0094 (14) | 0.0170 (16) | 0.0171 (14) | −0.0038 (11) | 0.0001 (11) | −0.0043 (12) |
| N1 | 0.0152 (17) | 0.0113 (18) | 0.0082 (15) | −0.0010 (13) | −0.0008 (13) | 0.0017 (13) |
| C1 | 0.013 (2) | 0.015 (2) | 0.0076 (18) | −0.0016 (16) | −0.0038 (15) | 0.0031 (16) |
| Pt2 | 0.01050 (9) | 0.00972 (10) | 0.01119 (9) | −0.00181 (6) | −0.00188 (6) | −0.00010 (6) |
| O2A | 0.0183 (15) | 0.0101 (15) | 0.0158 (14) | 0.0003 (12) | −0.0065 (11) | 0.0017 (11) |
| N2A | 0.0095 (16) | 0.0140 (19) | 0.0178 (18) | −0.0016 (13) | −0.0003 (13) | 0.0008 (14) |
| C2A | 0.015 (2) | 0.007 (2) | 0.0144 (19) | 0.0029 (16) | −0.0002 (16) | −0.0007 (16) |
| N2 | 0.0115 (17) | 0.0108 (18) | 0.0132 (16) | −0.0028 (13) | −0.0016 (13) | −0.0009 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0139 (14) | 0.0098 (15) | 0.0205 (15) | 0.0016 (11) | −0.0080 (12) | −0.0010 (12) |
| C2 | 0.013 (2) | 0.014 (2) | 0.015 (2) | −0.0046 (16) | −0.0009 (16) | −0.0032 (17) |
| C3A | 0.019 (2) | 0.014 (2) | 0.013 (2) | −0.0034 (17) | −0.0032 (16) | −0.0013 (16) |
| O3A | 0.0259 (17) | 0.0258 (18) | 0.0175 (15) | −0.0096 (14) | 0.0030 (13) | −0.0103 (13) |
| O3 | 0.0155 (15) | 0.0225 (17) | 0.0182 (15) | −0.0089 (13) | −0.0013 (12) | −0.0013 (12) |
| C3 | 0.0105 (19) | 0.009 (2) | 0.017 (2) | −0.0030 (15) | −0.0038 (16) | 0.0001 (16) |
| O4A | 0.0216 (16) | 0.0119 (16) | 0.0257 (16) | 0.0004 (12) | −0.0080 (13) | −0.0019 (13) |
| C4A | 0.014 (2) | 0.020 (2) | 0.014 (2) | 0.0002 (17) | −0.0005 (16) | −0.0025 (17) |
| O4 | 0.0226 (16) | 0.0088 (16) | 0.0288 (17) | −0.0007 (12) | −0.0121 (13) | 0.0030 (12) |
| C4 | 0.014 (2) | 0.017 (2) | 0.0122 (19) | −0.0004 (16) | −0.0015 (16) | 0.0007 (16) |
| C5A | 0.018 (2) | 0.025 (3) | 0.018 (2) | −0.0067 (18) | −0.0035 (17) | 0.0012 (18) |
| C5 | 0.017 (2) | 0.029 (3) | 0.013 (2) | 0.0005 (18) | −0.0033 (17) | −0.0067 (18) |
| O5 | 0.0225 (17) | 0.0217 (19) | 0.0295 (19) | −0.0084 (14) | 0.0011 (14) | −0.0052 (15) |
| C6A | 0.022 (2) | 0.017 (2) | 0.019 (2) | −0.0072 (18) | −0.0057 (18) | 0.0005 (18) |
| C6 | 0.020 (2) | 0.017 (2) | 0.020 (2) | −0.0005 (17) | −0.0083 (18) | −0.0037 (18) |
| O6 | 0.0273 (18) | 0.027 (2) | 0.0249 (18) | −0.0142 (15) | −0.0095 (15) | 0.0045 (15) |
| C7A | 0.012 (2) | 0.022 (2) | 0.016 (2) | −0.0033 (17) | −0.0019 (16) | 0.0016 (17) |
| C7 | 0.014 (2) | 0.016 (2) | 0.014 (2) | −0.0013 (16) | −0.0036 (16) | 0.0006 (16) |
| O7 | 0.0158 (17) | 0.044 (2) | 0.0187 (17) | 0.0070 (15) | −0.0038 (14) | −0.0091 (15) |
| C8 | 0.016 (2) | 0.019 (2) | 0.014 (2) | 0.0022 (17) | −0.0025 (16) | 0.0017 (17) |
| C8A | 0.017 (2) | 0.029 (3) | 0.020 (2) | −0.0005 (19) | −0.0056 (18) | 0.0079 (19) |
| O8 | 0.0190 (18) | 0.027 (2) | 0.0301 (19) | −0.0022 (15) | 0.0001 (14) | −0.0068 (16) |
| C9A | 0.017 (2) | 0.017 (2) | 0.029 (2) | 0.0001 (18) | −0.0030 (18) | 0.0074 (19) |
| C9 | 0.022 (2) | 0.015 (2) | 0.0115 (19) | 0.0080 (17) | −0.0041 (17) | 0.0019 (16) |
| C10A | 0.009 (2) | 0.018 (2) | 0.023 (2) | −0.0026 (16) | 0.0033 (16) | 0.0033 (18) |
| C10 | 0.021 (2) | 0.012 (2) | 0.0087 (19) | 0.0015 (16) | 0.0000 (16) | −0.0003 (15) |
| C11A | 0.0083 (18) | 0.007 (2) | 0.021 (2) | 0.0011 (15) | 0.0011 (16) | −0.0002 (16) |
| C11 | 0.015 (2) | 0.0052 (19) | 0.0086 (18) | 0.0006 (15) | −0.0012 (15) | 0.0012 (14) |
| C12A | 0.0066 (18) | 0.015 (2) | 0.015 (2) | −0.0026 (15) | 0.0013 (15) | −0.0007 (16) |
| C12 | 0.015 (2) | 0.014 (2) | 0.0080 (18) | 0.0002 (16) | −0.0008 (15) | −0.0003 (16) |
| C13A | 0.010 (2) | 0.017 (2) | 0.024 (2) | −0.0034 (16) | 0.0036 (17) | −0.0067 (18) |
| C13 | 0.019 (2) | 0.017 (2) | 0.0111 (19) | −0.0051 (17) | −0.0016 (16) | −0.0018 (16) |
| C14A | 0.015 (2) | 0.021 (2) | 0.026 (2) | −0.0024 (17) | −0.0017 (18) | −0.0123 (19) |
| C14 | 0.020 (2) | 0.017 (2) | 0.013 (2) | −0.0074 (17) | −0.0010 (16) | −0.0027 (16) |
| C15A | 0.017 (2) | 0.029 (3) | 0.016 (2) | −0.0014 (18) | −0.0031 (17) | −0.0067 (19) |
| C15 | 0.010 (2) | 0.026 (3) | 0.014 (2) | −0.0007 (17) | −0.0029 (16) | −0.0034 (17) |
| C16A | 0.013 (2) | 0.019 (2) | 0.016 (2) | −0.0009 (17) | −0.0011 (16) | −0.0015 (17) |
| C16 | 0.014 (2) | 0.013 (2) | 0.0121 (19) | 0.0029 (16) | −0.0009 (15) | −0.0017 (16) |
| C17A | 0.0064 (19) | 0.019 (2) | 0.031 (2) | −0.0013 (16) | 0.0015 (17) | 0.0135 (19) |
| C17 | 0.026 (2) | 0.012 (2) | 0.0102 (19) | −0.0051 (17) | 0.0010 (17) | −0.0039 (16) |
| C18A | 0.015 (2) | 0.013 (2) | 0.036 (3) | −0.0026 (17) | 0.0033 (19) | −0.0094 (19) |
| C18 | 0.024 (2) | 0.013 (2) | 0.015 (2) | −0.0076 (17) | −0.0043 (17) | −0.0015 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1A—C1A | 1.294 (5) | C6—H6A | 0.9900 |
| O1A—Pt2 | 2.012 (3) | C6—H6B | 0.9900 |
| N1A—C7A | 1.328 (5) | O6—H6V | 0.84 (2) |

| | | | |
|---|---|---|---|
| N1A—C11A | 1.368 (5) | O6—H6W | 0.83 (2) |
| N1A—Pt2 | 1.989 (3) | C7A—C8A | 1.400 (6) |
| C1A—O3A | 1.225 (5) | C7A—H7AA | 0.9500 |
| C1A—C3A | 1.534 (6) | C7—C8 | 1.394 (6) |
| Pt1—N1 | 1.992 (3) | C7—H7A | 0.9500 |
| Pt1—N2 | 1.996 (3) | O7—H7V | 0.83 (2) |
| Pt1—O2 | 2.000 (3) | O7—H7W | 0.83 (2) |
| Pt1—O1 | 2.010 (3) | C8—C9 | 1.378 (6) |
| O1—C1 | 1.290 (5) | C8—H8A | 0.9500 |
| N1—C7 | 1.333 (5) | C8A—C9A | 1.373 (7) |
| N1—C11 | 1.366 (5) | C8A—H8AA | 0.9500 |
| C1—O3 | 1.240 (5) | O8—H8V | 0.85 (2) |
| C1—C3 | 1.524 (5) | O8—H8W | 0.84 (2) |
| Pt2—N2A | 1.996 (3) | C9A—C10A | 1.402 (6) |
| Pt2—O2A | 2.000 (3) | C9A—H9AA | 0.9500 |
| O2A—C2A | 1.303 (5) | C9—C10 | 1.409 (6) |
| N2A—C16A | 1.330 (5) | C9—H9A | 0.9500 |
| N2A—C12A | 1.359 (5) | C10A—C11A | 1.410 (6) |
| C2A—O4A | 1.217 (5) | C10A—C17A | 1.466 (6) |
| C2A—C3A | 1.532 (6) | C10—C11 | 1.393 (6) |
| N2—C16 | 1.328 (5) | C10—C17 | 1.434 (6) |
| N2—C12 | 1.349 (5) | C11A—C12A | 1.422 (6) |
| O2—C2 | 1.296 (5) | C11—C12 | 1.423 (5) |
| C2—O4 | 1.224 (5) | C12A—C13A | 1.400 (6) |
| C2—C3 | 1.528 (5) | C12—C13 | 1.403 (6) |
| C3A—C6A | 1.541 (6) | C13A—C14A | 1.404 (6) |
| C3A—C4A | 1.560 (6) | C13A—C18A | 1.440 (6) |
| C3—C6 | 1.538 (6) | C13—C14 | 1.415 (6) |
| C3—C4 | 1.560 (5) | C13—C18 | 1.419 (6) |
| C4A—C5A | 1.548 (6) | C14A—C15A | 1.367 (6) |
| C4A—H4AA | 0.9900 | C14A—H14A | 0.9500 |
| C4A—H4AB | 0.9900 | C14—C15 | 1.374 (6) |
| C4—C5 | 1.545 (6) | C14—H14B | 0.9500 |
| C4—H4A | 0.9900 | C15A—C16A | 1.400 (6) |
| C4—H4B | 0.9900 | C15A—H15A | 0.9500 |
| C5A—C6A | 1.544 (6) | C15—C16 | 1.385 (6) |
| C5A—H5AA | 0.9900 | C15—H15B | 0.9500 |
| C5A—H5AB | 0.9900 | C16A—H16A | 0.9500 |
| C5—C6 | 1.548 (6) | C16—H16B | 0.9500 |
| C5—H5A | 0.9900 | C17A—C18A | 1.331 (6) |
| C5—H5B | 0.9900 | C17A—H17A | 0.9500 |
| O5—H5V | 0.85 (2) | C17—C18 | 1.379 (6) |
| O5—H5W | 0.84 (2) | C17—H17B | 0.9500 |
| C6A—H6AA | 0.9900 | C18A—H18A | 0.9500 |
| C6A—H6AB | 0.9900 | C18—H18B | 0.9500 |

| | | | |
|---|---|---|---|
| C1A—O1A—Pt2 | 121.2 (2) | H6AA—C6A—H6AB | 111.1 |
| C7A—N1A—C11A | 118.6 (4) | C3—C6—C5 | 89.3 (3) |

| | | | |
|---|---|---|---|
| C7A—N1A—Pt2 | 128.4 (3) | C3—C6—H6A | 113.8 |
| C11A—N1A—Pt2 | 112.9 (3) | C5—C6—H6A | 113.8 |
| O3A—C1A—O1A | 122.3 (4) | C3—C6—H6B | 113.8 |
| O3A—C1A—C3A | 120.5 (4) | C5—C6—H6B | 113.8 |
| O1A—C1A—C3A | 117.2 (3) | H6A—C6—H6B | 111.0 |
| N1—Pt1—N2 | 81.97 (13) | H6V—O6—H6W | 100 (6) |
| N1—Pt1—O2 | 173.29 (12) | N1A—C7A—C8A | 121.2 (4) |
| N2—Pt1—O2 | 92.66 (12) | N1A—C7A—H7AA | 119.4 |
| N1—Pt1—O1 | 93.57 (12) | C8A—C7A—H7AA | 119.4 |
| N2—Pt1—O1 | 174.96 (12) | N1—C7—C8 | 120.9 (4) |
| O2—Pt1—O1 | 91.63 (11) | N1—C7—H7A | 119.6 |
| C1—O1—Pt1 | 122.9 (2) | C8—C7—H7A | 119.6 |
| C7—N1—C11 | 118.9 (3) | H7V—O7—H7W | 107 (5) |
| C7—N1—Pt1 | 128.1 (3) | C9—C8—C7 | 120.9 (4) |
| C11—N1—Pt1 | 112.9 (3) | C9—C8—H8A | 119.5 |
| O3—C1—O1 | 120.5 (4) | C7—C8—H8A | 119.5 |
| O3—C1—C3 | 121.7 (4) | C9A—C8A—C7A | 120.4 (4) |
| O1—C1—C3 | 117.8 (3) | C9A—C8A—H8AA | 119.8 |
| N1A—Pt2—N2A | 82.27 (14) | C7A—C8A—H8AA | 119.8 |
| N1A—Pt2—O2A | 174.10 (12) | H8V—O8—H8W | 99 (6) |
| N2A—Pt2—O2A | 93.23 (12) | C8A—C9A—C10A | 120.2 (4) |
| N1A—Pt2—O1A | 93.17 (13) | C8A—C9A—H9AA | 119.9 |
| N2A—Pt2—O1A | 175.17 (12) | C10A—C9A—H9AA | 119.9 |
| O2A—Pt2—O1A | 91.21 (11) | C8—C9—C10 | 118.9 (4) |
| C2A—O2A—Pt2 | 120.2 (2) | C8—C9—H9A | 120.6 |
| C16A—N2A—C12A | 119.2 (4) | C10—C9—H9A | 120.6 |
| C16A—N2A—Pt2 | 128.1 (3) | C9A—C10A—C11A | 115.9 (4) |
| C12A—N2A—Pt2 | 112.6 (3) | C9A—C10A—C17A | 126.4 (4) |
| O4A—C2A—O2A | 122.4 (4) | C11A—C10A—C17A | 117.6 (4) |
| O4A—C2A—C3A | 120.5 (4) | C11—C10—C9 | 117.1 (4) |
| O2A—C2A—C3A | 117.0 (3) | C11—C10—C17 | 119.1 (4) |
| C16—N2—C12 | 119.0 (3) | C9—C10—C17 | 123.8 (4) |
| C16—N2—Pt1 | 128.0 (3) | N1A—C11A—C10A | 123.7 (4) |
| C12—N2—Pt1 | 113.0 (3) | N1A—C11A—C12A | 115.8 (4) |
| C2—O2—Pt1 | 121.2 (2) | C10A—C11A—C12A | 120.6 (4) |
| O4—C2—O2 | 121.5 (4) | N1—C11—C10 | 123.2 (4) |
| O4—C2—C3 | 120.3 (3) | N1—C11—C12 | 115.6 (3) |
| O2—C2—C3 | 118.2 (4) | C10—C11—C12 | 121.1 (4) |
| C2A—C3A—C1A | 108.4 (3) | N2A—C12A—C13A | 123.0 (4) |
| C2A—C3A—C6A | 116.8 (3) | N2A—C12A—C11A | 116.4 (3) |
| C1A—C3A—C6A | 113.5 (3) | C13A—C12A—C11A | 120.5 (4) |
| C2A—C3A—C4A | 116.7 (3) | N2—C12—C13 | 123.7 (4) |
| C1A—C3A—C4A | 111.6 (3) | N2—C12—C11 | 116.5 (3) |
| C6A—C3A—C4A | 88.8 (3) | C13—C12—C11 | 119.7 (4) |
| C1—C3—C2 | 109.7 (3) | C12A—C13A—C14A | 116.7 (4) |
| C1—C3—C6 | 114.4 (3) | C12A—C13A—C18A | 118.1 (4) |
| C2—C3—C6 | 116.1 (3) | C14A—C13A—C18A | 125.2 (4) |
| C1—C3—C4 | 109.0 (3) | C12—C13—C14 | 116.0 (4) |

| | | | |
|---|---|---|---|
| C2—C3—C4 | 117.5 (3) | C12—C13—C18 | 118.5 (4) |
| C6—C3—C4 | 88.8 (3) | C14—C13—C18 | 125.5 (4) |
| C5A—C4A—C3A | 88.0 (3) | C15A—C14A—C13A | 119.9 (4) |
| C5A—C4A—H4AA | 114.0 | C15A—C14A—H14A | 120.1 |
| C3A—C4A—H4AA | 114.0 | C13A—C14A—H14A | 120.1 |
| C5A—C4A—H4AB | 114.0 | C15—C14—C13 | 119.3 (4) |
| C3A—C4A—H4AB | 114.0 | C15—C14—H14B | 120.4 |
| H4AA—C4A—H4AB | 111.2 | C13—C14—H14B | 120.4 |
| C5—C4—C3 | 88.5 (3) | C14A—C15A—C16A | 120.2 (4) |
| C5—C4—H4A | 113.9 | C14A—C15A—H15A | 119.9 |
| C3—C4—H4A | 113.9 | C16A—C15A—H15A | 119.9 |
| C5—C4—H4B | 113.9 | C14—C15—C16 | 120.6 (4) |
| C3—C4—H4B | 113.9 | C14—C15—H15B | 119.7 |
| H4A—C4—H4B | 111.1 | C16—C15—H15B | 119.7 |
| C6A—C5A—C4A | 89.2 (3) | N2A—C16A—C15A | 121.0 (4) |
| C6A—C5A—H5AA | 113.8 | N2A—C16A—H16A | 119.5 |
| C4A—C5A—H5AA | 113.8 | C15A—C16A—H16A | 119.5 |
| C6A—C5A—H5AB | 113.8 | N2—C16—C15 | 121.3 (4) |
| C4A—C5A—H5AB | 113.8 | N2—C16—H16B | 119.3 |
| H5AA—C5A—H5AB | 111.0 | C15—C16—H16B | 119.3 |
| C4—C5—C6 | 89.0 (3) | C18A—C17A—C10A | 120.7 (4) |
| C4—C5—H5A | 113.8 | C18A—C17A—H17A | 119.7 |
| C6—C5—H5A | 113.8 | C10A—C17A—H17A | 119.7 |
| C4—C5—H5B | 113.8 | C18—C17—C10 | 119.2 (4) |
| C6—C5—H5B | 113.8 | C18—C17—H17B | 120.4 |
| H5A—C5—H5B | 111.0 | C10—C17—H17B | 120.4 |
| H5V—O5—H5W | 112 (6) | C17A—C18A—C13A | 122.4 (4) |
| C3A—C6A—C5A | 88.9 (3) | C17A—C18A—H18A | 118.8 |
| C3A—C6A—H6AA | 113.8 | C13A—C18A—H18A | 118.8 |
| C5A—C6A—H6AA | 113.8 | C17—C18—C13 | 122.3 (4) |
| C3A—C6A—H6AB | 113.8 | C17—C18—H18B | 118.8 |
| C5A—C6A—H6AB | 113.8 | C13—C18—H18B | 118.8 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5*W*···O6 | 0.84 | 1.97 | 2.802 (5) | 170 |
| O6—H6*W*···O3 | 0.83 | 2.03 | 2.842 (4) | 165 |
| O7—H7*W*···O3*A* | 0.83 | 1.93 | 2.753 (4) | 169 |
| O8—H8*V*···O7 | 0.85 | 1.95 | 2.806 (5) | 175 |
| O5—H5*V*···O8$^{i}$ | 0.85 | 1.98 | 2.821 (5) | 169 |
| O6—H6*V*···O4$^{ii}$ | 0.84 | 2.00 | 2.839 (4) | 173 |
| O7—H7*V*···O4*A*$^{iii}$ | 0.83 | 2.00 | 2.828 (4) | 176 |
| O8—H8*W*···O1$^{iv}$ | 0.84 | 2.43 | 3.125 (4) | 142 |
| O8—H8*W*···O3$^{iv}$ | 0.84 | 2.17 | 2.971 (4) | 160 |
| C7*A*—H7*AA*···O3$^{iv}$ | 0.95 | 2.55 | 3.376 (5) | 146 |
| C7—H7*A*···O7$^{iv}$ | 0.95 | 2.49 | 3.145 (5) | 126 |
| C8—H8*A*···O5$^{v}$ | 0.95 | 2.59 | 3.259 (6) | 128 |

| | | | | |
|---|---|---|---|---|
| C9—H9*A*···O6$^{v}$ | 0.95 | 2.51 | 3.436 (6) | 165 |
| C14*A*—H14*A*···O8$^{vi}$ | 0.95 | 2.35 | 3.230 (6) | 154 |
| C14—H14*B*···O5$^{vii}$ | 0.95 | 2.36 | 3.309 (6) | 174 |
| C18*A*—H18*A*···O4*A*$^{v}$ | 0.95 | 2.38 | 3.196 (5) | 144 |
| C18—H18*B*···O4$^{v}$ | 0.95 | 2.55 | 3.151 (5) | 121 |

Symmetry codes: (i) *x*+1, *y*, *z*−1; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+2, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, *y*−1, *z*; (vi) −*x*, −*y*+1, −*z*+1; (vii) *x*−1, *y*−1, *z*.