

catena-Poly[[$(18\text{-crown-6}\text{-}\kappa^6\text{O})$ -potassium]- μ -chlorido-[$(1\text{H}$ -benzotriazol-1-ol- $\kappa^3\text{N}^3)$ chloridoplatinum(II)]- μ -(benzotriazol-1-olato- $\kappa^2\text{N}^3\text{:O})$]

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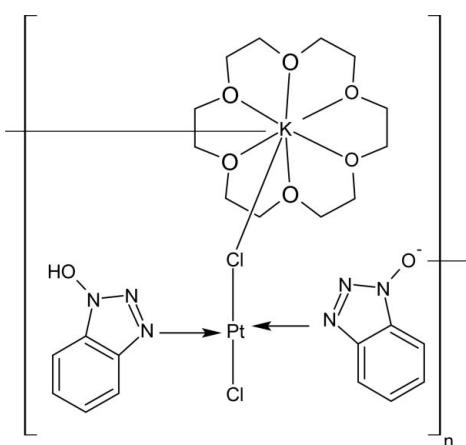
Received 25 April 2010; accepted 29 April 2010

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C-C}) = 0.023$ Å; R factor = 0.063; wR factor = 0.178; data-to-parameter ratio = 28.2.

In the structure of the title compound, $[\text{KPt}(\text{C}_6\text{H}_4\text{N}_3\text{O})\text{Cl}_2(\text{C}_6\text{H}_5\text{N}_3\text{O})(\text{C}_{12}\text{H}_{24}\text{O}_6)]$, the Pt^{II} atom is in a distorted square-planar geometry. The crystal structure is consolidated by O—H···O hydrogen bonds. The measured crystal was a non-merohedral twin with four components.

Related literature

For related literature, see Anderson *et al.* (1963). For related structures, see Bosch *et al.* (1983).



Experimental

Crystal data

| | |
|---|---|
| $[\text{KPt}(\text{C}_6\text{H}_4\text{N}_3\text{O})\text{Cl}_2(\text{C}_6\text{H}_5\text{N}_3\text{O})(\text{C}_{12}\text{H}_{24}\text{O}_6)]$ | $\beta = 99.249 (3)^\circ$ |
| $M_r = 838.65$ | $V = 3105.2 (5) \text{ \AA}^3$ |
| Monoclinic, $P2_1/c$ | $Z = 4$ |
| $a = 14.2727 (13) \text{ \AA}$ | Mo $K\alpha$ radiation |
| $b = 10.9821 (10) \text{ \AA}$ | $\mu = 4.88 \text{ mm}^{-1}$ |
| $c = 20.0716 (18) \text{ \AA}$ | $T = 173 \text{ K}$ |
| | $0.17 \times 0.10 \times 0.08 \text{ mm}$ |

Data collection

| | |
|---|--|
| Bruker SMART APEXII CCD diffractometer | 10775 measured reflections |
| Absorption correction: multi-scan (<i>TWINABS</i> ; Sheldrick, 1999) | 10775 independent reflections |
| $T_{\min} = 0.494$, $T_{\max} = 0.746$ | 9006 reflections with $I > 2\sigma(I)$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | 382 parameters |
| $wR(F^2) = 0.178$ | H-atom parameters constrained |
| $S = 1.07$ | $\Delta\rho_{\max} = 1.77 \text{ e \AA}^{-3}$ |
| 10775 reflections | $\Delta\rho_{\min} = -1.78 \text{ e \AA}^{-3}$ |

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

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| O20—H20···O10 ⁱ | 0.84 | 1.76 | 2.466 (12) | 141 |
| Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$. | | | | |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5255).

References

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supporting information

Acta Cryst. (2010). E66, m631 [https://doi.org/10.1107/S1600536810015898]



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S1. Comment

For related literature, see Anderson *et al.* (1963) and for related structures see Bosch *et al.* (1983).

The metal platinum exhibits the distorted square planar coordination geometry. The geometry is completed by two chlorine atoms and two nitrogen atoms from the 1-oxobenzotriazole ligands. Distortion in the square-planar Pt coordination sphere is signaled by angles about Pt ranging from 88.9 (3) Å to 91.2 (3) Å. The K ion is coordinated by six oxygen atoms of the crown ether and also by one terminal Cl atom attached to the metal platinum and one O atom from the 1-oxobenzotriazole ligand forming a hexagonal pyramid. The potassium ion lies in the plane of the 18-crown 6-molecule, with mean K—O distance of 2.8 Å.

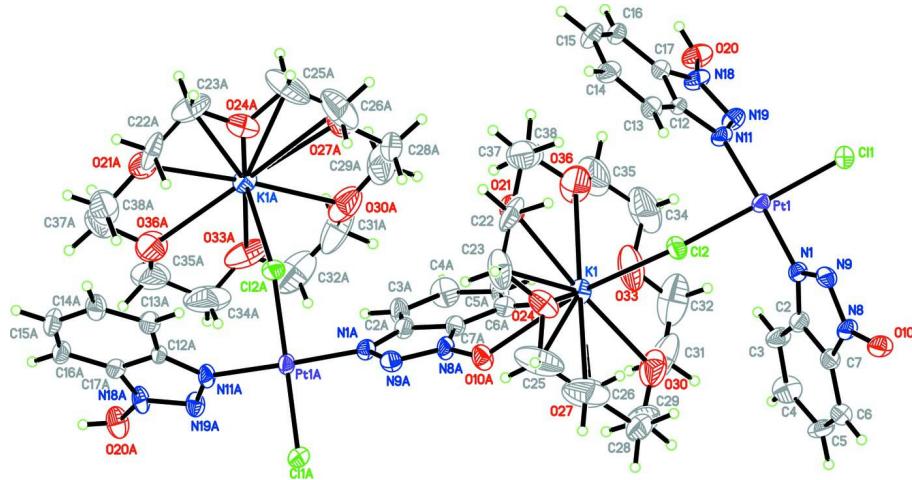
The crystal structure is consolidated by O—H···O hydrogen bonds.

S2. Experimental

A mixture of potassium tetrachloroplatinate(II) (0.0208 g, 0.05 mmol) and 1-hydroxybenzotriazole (0.0135 g, 0.1 mmol) 18-crown-6 ether (0.013 g 0.05 mmol) in acetone (15 ml) was heated at 313 K with stirring for 30 min. The yellow colour compound formed was filtered off, and dried. The compound was then dissolved in dichloromethane and kept at 278 K. Pale yellow crystals are formed after one month on slow evaporation.

S3. Refinement

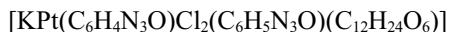
All H atoms were positioned geometrically with C—H=0.95 Å (aromatic) C—H=0.98 Å (methylene), O—H= 0.84 Å and refined using a riding model with, $U_{\text{iso}}(\text{H})=1.2U_{\text{equ}}(\text{C})$ and $1.5U_{\text{equ}}(\text{O})$. The measured crystal was a non-merohedral twin with four components 0.536 (1) 0.194 (2), 0.226 (1) and 0.044 (1).

**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme.

catena-Poly[[$(18\text{-crown-6}\text{-}\kappa^6\text{O})$]potassium]- μ -chlorido- [$(1H\text{-benzotriazol-1-ol-}\kappa\text{N}^3)$]chloridoplatinum(II)]- μ -(benzotriazol-1-olato- $\kappa^2\text{N}^3\text{:O}$)]

Crystal data



$M_r = 838.65$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.2727 (13)$ Å

$b = 10.9821 (10)$ Å

$c = 20.0716 (18)$ Å

$\beta = 99.249 (3)^\circ$

$V = 3105.2 (5)$ Å³

$Z = 4$

$F(000) = 1656$

$D_x = 1.794 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 8964 reflections

$\theta = 2.3\text{--}26.9^\circ$

$\mu = 4.88 \text{ mm}^{-1}$

$T = 173$ K

Block, light yellow

$0.17 \times 0.10 \times 0.08$ mm

Data collection

Bruker SMART CCD

diffractometer

Radiation source: sealed Tube

Graphite monochromator

CCD scan

Absorption correction: multi-scan
(TWINABS; Sheldrick, 1999)

$T_{\min} = 0.494$, $T_{\max} = 0.746$

10775 measured reflections

10775 independent reflections

9006 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 1.5^\circ$

$h = -18 \rightarrow 18$

$k = 0 \rightarrow 14$

$l = 0 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.178$

$S = 1.07$

10775 reflections

382 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0972P)^2 + 18.2058P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.77 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.78 \text{ e } \text{\AA}^{-3}$$

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.

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 $h F^2 > \sigma(F^2)$ 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. Crystal was split into 4 fragments and refined using HKLF 5/BASF method'

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|---------------|----------------------------------|
| Pt1 | 0.26231 (3) | 0.37872 (3) | 0.527664 (17) | 0.02221 (11) |
| Cl1 | 0.2212 (2) | 0.2066 (3) | 0.58061 (15) | 0.0375 (7) |
| Cl2 | 0.3097 (2) | 0.5510 (2) | 0.47650 (14) | 0.0352 (6) |
| N1 | 0.2340 (6) | 0.4823 (8) | 0.6036 (4) | 0.0229 (17) |
| C2 | 0.1620 (8) | 0.5710 (9) | 0.5966 (5) | 0.025 (2) |
| C3 | 0.0955 (8) | 0.6111 (11) | 0.5421 (5) | 0.033 (2) |
| H3 | 0.0940 | 0.5768 | 0.4985 | 0.040* |
| C4 | 0.0340 (8) | 0.6989 (12) | 0.5523 (7) | 0.042 (3) |
| H4 | -0.0100 | 0.7293 | 0.5156 | 0.051* |
| C5 | 0.0348 (10) | 0.7488 (11) | 0.6216 (7) | 0.039 (3) |
| H5 | -0.0113 | 0.8079 | 0.6284 | 0.047* |
| C6 | 0.0992 (9) | 0.7126 (10) | 0.6750 (6) | 0.033 (2) |
| H6 | 0.1018 | 0.7468 | 0.7188 | 0.039* |
| C7 | 0.1626 (8) | 0.6199 (10) | 0.6609 (5) | 0.026 (2) |
| N8 | 0.2308 (7) | 0.5555 (8) | 0.7023 (4) | 0.0261 (18) |
| N9 | 0.2737 (7) | 0.4742 (8) | 0.6659 (4) | 0.0281 (19) |
| O10 | 0.2552 (6) | 0.5648 (7) | 0.7691 (4) | 0.0341 (18) |
| N11 | 0.2852 (7) | 0.2812 (8) | 0.4469 (4) | 0.0256 (19) |
| C12 | 0.3658 (7) | 0.2703 (9) | 0.4180 (5) | 0.022 (2) |
| C13 | 0.4600 (9) | 0.3121 (10) | 0.4392 (5) | 0.029 (2) |
| H13 | 0.4781 | 0.3549 | 0.4804 | 0.035* |
| C14 | 0.5228 (9) | 0.2866 (11) | 0.3965 (6) | 0.034 (3) |
| H14 | 0.5870 | 0.3119 | 0.4081 | 0.040* |
| C15 | 0.4941 (9) | 0.2230 (12) | 0.3349 (6) | 0.038 (3) |
| H15 | 0.5403 | 0.2078 | 0.3067 | 0.045* |
| C16 | 0.4049 (9) | 0.1832 (10) | 0.3144 (6) | 0.030 (2) |
| H16 | 0.3864 | 0.1416 | 0.2728 | 0.036* |
| C17 | 0.3423 (8) | 0.2076 (9) | 0.3586 (5) | 0.028 (2) |
| N18 | 0.2459 (7) | 0.1814 (9) | 0.3558 (4) | 0.031 (2) |
| N19 | 0.2129 (6) | 0.2248 (8) | 0.4094 (4) | 0.0274 (19) |
| O20 | 0.1871 (6) | 0.1243 (9) | 0.3072 (4) | 0.0410 (19) |

| | | | | |
|------|--------------|-------------|--------------|------------|
| H20 | 0.2188 | 0.0847 | 0.2828 | 0.062* |
| O21 | 0.4161 (7) | 0.6331 (9) | 0.3022 (5) | 0.047 (2) |
| C22 | 0.4979 (11) | 0.6571 (17) | 0.3516 (7) | 0.056 (4) |
| H22A | 0.4980 | 0.6022 | 0.3907 | 0.067* |
| H22B | 0.5561 | 0.6407 | 0.3320 | 0.067* |
| C23 | 0.4981 (11) | 0.7788 (17) | 0.3731 (9) | 0.060 (5) |
| H23A | 0.5588 | 0.7971 | 0.4028 | 0.073* |
| H23B | 0.4923 | 0.8336 | 0.3335 | 0.073* |
| O24 | 0.4228 (7) | 0.7993 (8) | 0.4081 (5) | 0.041 (2) |
| C25 | 0.4190 (14) | 0.9189 (16) | 0.4377 (13) | 0.084 (7) |
| H25A | 0.4796 | 0.9350 | 0.4680 | 0.100* |
| H25B | 0.4119 | 0.9808 | 0.4014 | 0.100* |
| C26 | 0.3432 (19) | 0.9305 (19) | 0.4746 (11) | 0.093 (7) |
| H26A | 0.3465 | 1.0111 | 0.4969 | 0.111* |
| H26B | 0.3490 | 0.8672 | 0.5101 | 0.111* |
| O27 | 0.2539 (9) | 0.9180 (9) | 0.4314 (5) | 0.058 (3) |
| C28 | 0.1692 (19) | 0.9269 (17) | 0.4658 (11) | 0.085 (7) |
| H28A | 0.1752 | 0.8691 | 0.5041 | 0.103* |
| H28B | 0.1639 | 1.0103 | 0.4835 | 0.103* |
| C29 | 0.084 (2) | 0.897 (2) | 0.4162 (15) | 0.108 (10) |
| H29A | 0.0261 | 0.9117 | 0.4364 | 0.129* |
| H29B | 0.0813 | 0.9504 | 0.3760 | 0.129* |
| O30 | 0.0883 (8) | 0.7821 (13) | 0.3984 (6) | 0.072 (4) |
| C31 | 0.0019 (12) | 0.740 (3) | 0.3545 (10) | 0.090 (8) |
| H31A | -0.0530 | 0.7486 | 0.3787 | 0.108* |
| H31B | -0.0100 | 0.7918 | 0.3137 | 0.108* |
| C32 | 0.0092 (14) | 0.613 (3) | 0.3341 (10) | 0.092 (8) |
| H32A | 0.0174 | 0.5602 | 0.3746 | 0.111* |
| H32B | -0.0504 | 0.5886 | 0.3048 | 0.111* |
| O33 | 0.0817 (8) | 0.5961 (12) | 0.3011 (6) | 0.072 (4) |
| C34 | 0.0933 (18) | 0.468 (2) | 0.2871 (12) | 0.096 (8) |
| H34A | 0.0316 | 0.4331 | 0.2665 | 0.115* |
| H34B | 0.1158 | 0.4242 | 0.3297 | 0.115* |
| C35 | 0.1637 (17) | 0.4551 (19) | 0.2400 (11) | 0.092 (7) |
| H35A | 0.1704 | 0.3682 | 0.2285 | 0.110* |
| H35B | 0.1420 | 0.5006 | 0.1978 | 0.110* |
| O36 | 0.2516 (10) | 0.5015 (11) | 0.2723 (6) | 0.074 (4) |
| C37 | 0.3247 (16) | 0.4920 (14) | 0.2324 (8) | 0.072 (6) |
| H37A | 0.3163 | 0.5539 | 0.1960 | 0.086* |
| H37B | 0.3247 | 0.4102 | 0.2117 | 0.086* |
| C38 | 0.4148 (16) | 0.5133 (16) | 0.2799 (8) | 0.069 (5) |
| H38A | 0.4188 | 0.4571 | 0.3189 | 0.083* |
| H38B | 0.4699 | 0.4980 | 0.2568 | 0.083* |
| K1 | 0.25264 (18) | 0.7160 (2) | 0.34906 (12) | 0.0318 (5) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|---------------|
| Pt1 | 0.02707 (18) | 0.02415 (16) | 0.01630 (15) | 0.0034 (2) | 0.00617 (14) | -0.00098 (16) |
| C11 | 0.0513 (18) | 0.0285 (13) | 0.0382 (15) | 0.0003 (12) | 0.0242 (14) | 0.0044 (12) |
| C12 | 0.0531 (17) | 0.0260 (12) | 0.0287 (13) | -0.0019 (12) | 0.0135 (12) | 0.0038 (11) |
| N1 | 0.026 (4) | 0.025 (4) | 0.018 (4) | 0.005 (3) | 0.004 (3) | 0.004 (3) |
| C2 | 0.027 (5) | 0.028 (5) | 0.023 (5) | 0.002 (4) | 0.007 (4) | 0.000 (4) |
| C3 | 0.043 (6) | 0.035 (6) | 0.022 (5) | 0.014 (5) | 0.005 (4) | 0.000 (5) |
| C4 | 0.018 (5) | 0.051 (8) | 0.055 (8) | 0.014 (5) | -0.003 (5) | 0.009 (6) |
| C5 | 0.045 (7) | 0.033 (6) | 0.041 (7) | 0.015 (5) | 0.016 (6) | -0.005 (5) |
| C6 | 0.037 (6) | 0.026 (5) | 0.037 (6) | -0.001 (5) | 0.013 (5) | 0.000 (5) |
| C7 | 0.036 (6) | 0.025 (4) | 0.019 (4) | -0.002 (5) | 0.005 (4) | -0.001 (4) |
| N8 | 0.036 (5) | 0.030 (5) | 0.013 (4) | 0.004 (4) | 0.005 (3) | -0.002 (3) |
| N9 | 0.037 (5) | 0.024 (4) | 0.023 (4) | 0.007 (4) | 0.004 (4) | 0.007 (3) |
| O10 | 0.049 (5) | 0.031 (4) | 0.021 (4) | 0.008 (4) | 0.002 (3) | -0.002 (3) |
| N11 | 0.035 (5) | 0.029 (4) | 0.013 (4) | 0.006 (4) | 0.004 (3) | -0.003 (3) |
| C12 | 0.030 (5) | 0.019 (4) | 0.020 (4) | 0.003 (4) | 0.011 (4) | 0.001 (4) |
| C13 | 0.037 (6) | 0.031 (5) | 0.018 (5) | -0.002 (5) | 0.002 (5) | -0.002 (4) |
| C14 | 0.031 (6) | 0.037 (6) | 0.034 (6) | 0.009 (5) | 0.007 (5) | -0.001 (5) |
| C15 | 0.041 (7) | 0.048 (7) | 0.027 (6) | 0.001 (6) | 0.016 (5) | -0.006 (5) |
| C16 | 0.039 (6) | 0.031 (5) | 0.023 (5) | 0.006 (5) | 0.013 (5) | 0.003 (4) |
| C17 | 0.029 (6) | 0.023 (5) | 0.033 (5) | 0.001 (4) | 0.013 (5) | 0.001 (4) |
| N18 | 0.040 (6) | 0.036 (5) | 0.016 (4) | 0.003 (4) | 0.001 (4) | -0.013 (4) |
| N19 | 0.028 (5) | 0.035 (5) | 0.020 (4) | -0.002 (4) | 0.002 (3) | -0.009 (4) |
| O20 | 0.043 (5) | 0.049 (5) | 0.028 (4) | 0.010 (5) | -0.003 (3) | -0.011 (4) |
| O21 | 0.057 (6) | 0.047 (5) | 0.038 (4) | 0.003 (5) | 0.010 (4) | 0.009 (4) |
| C22 | 0.051 (8) | 0.094 (13) | 0.028 (6) | 0.019 (8) | 0.023 (6) | 0.009 (7) |
| C23 | 0.033 (7) | 0.081 (12) | 0.066 (10) | -0.005 (8) | 0.004 (7) | 0.035 (9) |
| O24 | 0.045 (5) | 0.033 (4) | 0.040 (5) | -0.004 (4) | -0.014 (4) | 0.006 (4) |
| C25 | 0.067 (12) | 0.041 (8) | 0.127 (19) | -0.007 (8) | -0.032 (12) | -0.025 (10) |
| C26 | 0.13 (2) | 0.058 (11) | 0.084 (14) | 0.005 (13) | -0.008 (15) | -0.035 (10) |
| O27 | 0.094 (9) | 0.038 (5) | 0.047 (6) | 0.015 (5) | 0.025 (6) | -0.002 (4) |
| C28 | 0.14 (2) | 0.049 (9) | 0.084 (14) | -0.011 (11) | 0.081 (15) | -0.017 (9) |
| C29 | 0.13 (2) | 0.090 (17) | 0.13 (2) | 0.052 (16) | 0.086 (19) | 0.021 (16) |
| O30 | 0.052 (7) | 0.093 (9) | 0.079 (8) | 0.027 (6) | 0.032 (6) | 0.037 (7) |
| C31 | 0.031 (9) | 0.19 (3) | 0.051 (10) | 0.021 (12) | 0.012 (7) | 0.019 (14) |
| C32 | 0.054 (11) | 0.16 (3) | 0.055 (11) | -0.038 (15) | 0.001 (8) | 0.004 (14) |
| O33 | 0.045 (6) | 0.095 (10) | 0.075 (8) | -0.024 (6) | 0.001 (5) | 0.035 (7) |
| C34 | 0.111 (18) | 0.077 (14) | 0.096 (16) | -0.060 (13) | 0.008 (14) | 0.005 (12) |
| C35 | 0.125 (19) | 0.064 (12) | 0.091 (15) | -0.052 (13) | 0.031 (14) | -0.018 (11) |
| O36 | 0.098 (10) | 0.071 (8) | 0.060 (7) | -0.047 (7) | 0.027 (7) | -0.031 (6) |
| C37 | 0.137 (19) | 0.041 (8) | 0.039 (8) | -0.007 (10) | 0.021 (10) | -0.013 (6) |
| C38 | 0.106 (15) | 0.058 (10) | 0.045 (9) | 0.026 (10) | 0.016 (9) | 0.007 (7) |
| K1 | 0.0270 (12) | 0.0395 (13) | 0.0281 (11) | -0.0044 (10) | 0.0020 (9) | -0.0003 (10) |

Geometric parameters (\AA , \textdegree)

| | | | |
|---------------------|------------|----------------------|------------|
| Pt1—N1 | 1.996 (8) | C23—H23A | 0.9900 |
| Pt1—N11 | 2.013 (8) | C23—H23B | 0.9900 |
| Pt1—Cl1 | 2.290 (3) | O24—C25 | 1.446 (19) |
| Pt1—Cl2 | 2.306 (3) | O24—K1 | 2.687 (9) |
| Cl2—K1 | 3.133 (4) | C25—C26 | 1.41 (3) |
| N1—N9 | 1.290 (12) | C25—K1 | 3.523 (16) |
| N1—C2 | 1.407 (13) | C25—H25A | 0.9900 |
| C2—C7 | 1.396 (13) | C25—H25B | 0.9900 |
| C2—C3 | 1.399 (15) | C26—O27 | 1.43 (3) |
| C3—C4 | 1.341 (16) | C26—K1 | 3.538 (19) |
| C3—H3 | 0.9500 | C26—H26A | 0.9900 |
| C4—C5 | 1.492 (19) | C26—H26B | 0.9900 |
| C4—H4 | 0.9500 | O27—C28 | 1.49 (2) |
| C5—C6 | 1.355 (18) | O27—K1 | 2.764 (10) |
| C5—H5 | 0.9500 | C28—C29 | 1.48 (4) |
| C6—C7 | 1.421 (15) | C28—H28A | 0.9900 |
| C6—H6 | 0.9500 | C28—H28B | 0.9900 |
| C7—N8 | 1.371 (14) | C29—O30 | 1.32 (3) |
| N8—O10 | 1.334 (11) | C29—H29A | 0.9900 |
| N8—N9 | 1.360 (12) | C29—H29B | 0.9900 |
| O10—K1 ⁱ | 2.897 (8) | O30—C31 | 1.47 (2) |
| N11—N19 | 1.329 (13) | O30—K1 | 2.785 (11) |
| N11—C12 | 1.374 (13) | C31—C32 | 1.46 (3) |
| C12—C17 | 1.371 (14) | C31—H31A | 0.9900 |
| C12—C13 | 1.420 (16) | C31—H31B | 0.9900 |
| C13—C14 | 1.366 (16) | C32—O33 | 1.33 (2) |
| C13—H13 | 0.9500 | C32—H32A | 0.9900 |
| C14—C15 | 1.422 (17) | C32—H32B | 0.9900 |
| C14—H14 | 0.9500 | O33—C34 | 1.44 (3) |
| C15—C16 | 1.346 (18) | O33—K1 | 2.804 (11) |
| C15—H15 | 0.9500 | C34—C35 | 1.49 (3) |
| C16—C17 | 1.382 (14) | C34—H34A | 0.9900 |
| C16—H16 | 0.9500 | C34—H34B | 0.9900 |
| C17—N18 | 1.398 (15) | C35—O36 | 1.41 (2) |
| N18—N19 | 1.331 (12) | C35—H35A | 0.9900 |
| N18—O20 | 1.336 (12) | C35—H35B | 0.9900 |
| O20—H20 | 0.8400 | O36—C37 | 1.42 (2) |
| O21—C38 | 1.39 (2) | O36—K1 | 2.814 (11) |
| O21—C22 | 1.430 (18) | C37—C38 | 1.49 (3) |
| O21—K1 | 2.804 (10) | C37—H37A | 0.9900 |
| C22—C23 | 1.41 (2) | C37—H37B | 0.9900 |
| C22—H22A | 0.9900 | C38—H38A | 0.9900 |
| C22—H22B | 0.9900 | C38—H38B | 0.9900 |
| C23—O24 | 1.393 (19) | K1—O10 ⁱⁱ | 2.897 (8) |
| C23—K1 | 3.527 (15) | | |

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| N1—Pt1—N11 | 176.3 (3) | H28A—C28—H28B | 108.4 |
| N1—Pt1—Cl1 | 91.0 (3) | O30—C29—C28 | 109 (2) |
| N11—Pt1—Cl1 | 91.2 (3) | O30—C29—H29A | 109.9 |
| N1—Pt1—Cl2 | 89.0 (3) | C28—C29—H29A | 109.9 |
| N11—Pt1—Cl2 | 88.9 (3) | O30—C29—H29B | 109.9 |
| Cl1—Pt1—Cl2 | 177.77 (12) | C28—C29—H29B | 109.9 |
| Pt1—Cl2—K1 | 141.43 (13) | H29A—C29—H29B | 108.3 |
| N9—N1—C2 | 110.2 (8) | C29—O30—C31 | 113 (2) |
| N9—N1—Pt1 | 126.1 (7) | C29—O30—K1 | 115.1 (13) |
| C2—N1—Pt1 | 123.6 (7) | C31—O30—K1 | 112.2 (10) |
| C7—C2—C3 | 120.3 (10) | C32—C31—O30 | 112.2 (16) |
| C7—C2—N1 | 106.1 (9) | C32—C31—H31A | 109.2 |
| C3—C2—N1 | 133.5 (9) | O30—C31—H31A | 109.2 |
| C4—C3—C2 | 118.9 (11) | C32—C31—H31B | 109.2 |
| C4—C3—H3 | 120.5 | O30—C31—H31B | 109.2 |
| C2—C3—H3 | 120.5 | H31A—C31—H31B | 107.9 |
| C3—C4—C5 | 120.0 (11) | O33—C32—C31 | 111.7 (18) |
| C3—C4—H4 | 120.0 | O33—C32—H32A | 109.3 |
| C5—C4—H4 | 120.0 | C31—C32—H32A | 109.3 |
| C6—C5—C4 | 122.2 (11) | O33—C32—H32B | 109.3 |
| C6—C5—H5 | 118.9 | C31—C32—H32B | 109.3 |
| C4—C5—H5 | 118.9 | H32A—C32—H32B | 108.0 |
| C5—C6—C7 | 115.1 (11) | C32—O33—C34 | 110.8 (17) |
| C5—C6—H6 | 122.4 | C32—O33—K1 | 117.9 (13) |
| C7—C6—H6 | 122.4 | C34—O33—K1 | 113.7 (12) |
| N8—C7—C2 | 105.1 (9) | O33—C34—C35 | 109.2 (15) |
| N8—C7—C6 | 131.4 (9) | O33—C34—H34A | 109.9 |
| C2—C7—C6 | 123.4 (10) | C35—C34—H34A | 109.9 |
| O10—N8—N9 | 121.5 (9) | O33—C34—H34B | 109.9 |
| O10—N8—C7 | 128.0 (9) | C35—C34—H34B | 109.9 |
| N9—N8—C7 | 110.5 (8) | H34A—C34—H34B | 108.3 |
| N1—N9—N8 | 108.0 (8) | O36—C35—C34 | 108.2 (17) |
| N8—O10—K1 ⁱ | 126.6 (6) | O36—C35—H35A | 110.1 |
| N19—N11—C12 | 110.3 (8) | C34—C35—H35A | 110.1 |
| N19—N11—Pt1 | 119.5 (7) | O36—C35—H35B | 110.1 |
| C12—N11—Pt1 | 129.9 (7) | C34—C35—H35B | 110.1 |
| C17—C12—N11 | 107.9 (9) | H35A—C35—H35B | 108.4 |
| C17—C12—C13 | 120.7 (9) | C35—O36—C37 | 113.3 (13) |
| N11—C12—C13 | 131.4 (9) | C35—O36—K1 | 118.7 (12) |
| C14—C13—C12 | 115.5 (10) | C37—O36—K1 | 115.5 (9) |
| C14—C13—H13 | 122.3 | O36—C37—C38 | 105.3 (12) |
| C12—C13—H13 | 122.3 | O36—C37—H37A | 110.7 |
| C13—C14—C15 | 121.4 (12) | C38—C37—H37A | 110.7 |
| C13—C14—H14 | 119.3 | O36—C37—H37B | 110.7 |
| C15—C14—H14 | 119.3 | C38—C37—H37B | 110.7 |
| C16—C15—C14 | 123.5 (11) | H37A—C37—H37B | 108.8 |
| C16—C15—H15 | 118.3 | O21—C38—C37 | 108.6 (14) |
| C14—C15—H15 | 118.3 | O21—C38—H38A | 110.0 |

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| C15—C16—C17 | 114.6 (11) | C37—C38—H38A | 110.0 |
| C15—C16—H16 | 122.7 | O21—C38—H38B | 110.0 |
| C17—C16—H16 | 122.7 | C37—C38—H38B | 110.0 |
| C12—C17—C16 | 124.3 (11) | H38A—C38—H38B | 108.3 |
| C12—C17—N18 | 103.8 (9) | O24—K1—O27 | 62.9 (3) |
| C16—C17—N18 | 131.9 (11) | O24—K1—O30 | 120.5 (4) |
| N19—N18—O20 | 119.6 (9) | O27—K1—O30 | 60.2 (4) |
| N19—N18—C17 | 111.6 (9) | O24—K1—O33 | 170.7 (3) |
| O20—N18—C17 | 128.7 (9) | O27—K1—O33 | 120.3 (4) |
| N11—N19—N18 | 106.3 (8) | O30—K1—O33 | 60.5 (4) |
| N18—O20—H20 | 109.5 | O24—K1—O21 | 61.1 (3) |
| C38—O21—C22 | 111.3 (13) | O27—K1—O21 | 122.3 (4) |
| C38—O21—K1 | 116.5 (11) | O30—K1—O21 | 176.1 (4) |
| C22—O21—K1 | 109.8 (7) | O33—K1—O21 | 117.2 (4) |
| C23—C22—O21 | 110.4 (13) | O24—K1—O36 | 116.9 (4) |
| C23—C22—H22A | 109.6 | O27—K1—O36 | 176.5 (4) |
| O21—C22—H22A | 109.6 | O30—K1—O36 | 118.8 (4) |
| C23—C22—H22B | 109.6 | O33—K1—O36 | 59.4 (4) |
| O21—C22—H22B | 109.6 | O21—K1—O36 | 58.4 (3) |
| H22A—C22—H22B | 108.1 | O24—K1—O10 ⁱⁱ | 82.6 (3) |
| O24—C23—C22 | 110.2 (13) | O27—K1—O10 ⁱⁱ | 70.4 (3) |
| C22—C23—K1 | 79.6 (9) | O30—K1—O10 ⁱⁱ | 93.8 (3) |
| O24—C23—H23A | 109.6 | O33—K1—O10 ⁱⁱ | 106.7 (3) |
| C22—C23—H23A | 109.6 | O21—K1—O10 ⁱⁱ | 89.9 (3) |
| K1—C23—H23A | 151.2 | O36—K1—O10 ⁱⁱ | 113.1 (3) |
| O24—C23—H23B | 109.6 | O24—K1—Cl2 | 74.9 (2) |
| C22—C23—H23B | 109.6 | O27—K1—Cl2 | 90.0 (2) |
| K1—C23—H23B | 93.2 | O30—K1—Cl2 | 89.1 (2) |
| H23A—C23—H23B | 108.1 | O33—K1—Cl2 | 96.1 (2) |
| C23—O24—C25 | 115.9 (14) | O21—K1—Cl2 | 88.0 (2) |
| C23—O24—K1 | 116.0 (9) | O36—K1—Cl2 | 86.6 (3) |
| C25—O24—K1 | 113.5 (10) | O10 ⁱⁱ —K1—Cl2 | 155.23 (19) |
| C26—C25—O24 | 112.3 (16) | O24—K1—C25 | 22.1 (4) |
| C26—C25—K1 | 79.1 (11) | O27—K1—C25 | 41.5 (5) |
| C26—C25—H25A | 109.1 | O30—K1—C25 | 101.2 (5) |
| O24—C25—H25A | 109.1 | O33—K1—C25 | 161.7 (5) |
| K1—C25—H25A | 151.0 | O21—K1—C25 | 81.1 (4) |
| C26—C25—H25B | 109.1 | O36—K1—C25 | 138.6 (5) |
| O24—C25—H25B | 109.1 | O10 ⁱⁱ —K1—C25 | 71.7 (4) |
| K1—C25—H25B | 94.7 | Cl2—K1—C25 | 83.6 (4) |
| H25A—C25—H25B | 107.9 | O24—K1—C23 | 20.8 (4) |
| C25—C26—O27 | 111.0 (17) | O27—K1—C23 | 81.4 (4) |
| C25—C26—K1 | 77.9 (10) | O30—K1—C23 | 140.8 (5) |
| O27—C26—K1 | 46.8 (7) | O33—K1—C23 | 158.4 (5) |
| C25—C26—H26A | 109.4 | O21—K1—C23 | 41.2 (4) |
| O27—C26—H26A | 109.4 | O36—K1—C23 | 99.0 (4) |
| K1—C26—H26A | 154.5 | O10 ⁱⁱ —K1—C23 | 79.2 (3) |
| C25—C26—H26B | 109.4 | Cl2—K1—C23 | 83.1 (3) |

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| O27—C26—H26B | 109.4 | C25—K1—C23 | 39.9 (5) |
| K1—C26—H26B | 91.4 | O24—K1—C26 | 42.1 (5) |
| H26A—C26—H26B | 108.0 | O27—K1—C26 | 22.1 (5) |
| C26—O27—C28 | 115.1 (16) | O30—K1—C26 | 78.8 (5) |
| C26—O27—K1 | 111.1 (9) | O33—K1—C26 | 139.1 (5) |
| C28—O27—K1 | 113.7 (10) | O21—K1—C26 | 103.1 (5) |
| C29—C28—O27 | 108.3 (15) | O36—K1—C26 | 156.4 (5) |
| C29—C28—H28A | 110.0 | O10 ⁱⁱ —K1—C26 | 78.8 (4) |
| O27—C28—H28A | 110.0 | Cl2—K1—C26 | 77.7 (4) |
| C29—C28—H28B | 110.0 | C25—K1—C26 | 23.1 (5) |
| O27—C28—H28B | 110.0 | C23—K1—C26 | 62.0 (5) |
| | | | |
| N1—Pt1—Cl2—K1 | -113.6 (3) | C31—O30—K1—O33 | -17.8 (13) |
| N11—Pt1—Cl2—K1 | 63.3 (3) | C29—O30—K1—O36 | -161.1 (17) |
| Cl1—Pt1—N1—N9 | 59.4 (9) | C31—O30—K1—O36 | -29.7 (14) |
| Cl2—Pt1—N1—N9 | -118.4 (9) | C29—O30—K1—O10 ⁱⁱ | -42.1 (17) |
| Cl1—Pt1—N1—C2 | -116.4 (8) | C31—O30—K1—O10 ⁱⁱ | 89.3 (13) |
| Cl2—Pt1—N1—C2 | 65.8 (8) | C29—O30—K1—Cl2 | 113.3 (17) |
| N9—N1—C2—C7 | 1.6 (12) | C31—O30—K1—Cl2 | -115.3 (13) |
| Pt1—N1—C2—C7 | 178.0 (7) | C29—O30—K1—C25 | 30.0 (18) |
| N9—N1—C2—C3 | -176.5 (13) | C31—O30—K1—C25 | 161.4 (13) |
| Pt1—N1—C2—C3 | -0.1 (17) | C29—O30—K1—C23 | 35.5 (19) |
| C7—C2—C3—C4 | 1.4 (18) | C31—O30—K1—C23 | 166.9 (13) |
| N1—C2—C3—C4 | 179.2 (12) | C29—O30—K1—C26 | 35.7 (17) |
| C2—C3—C4—C5 | -2.3 (19) | C31—O30—K1—C26 | 167.1 (14) |
| C3—C4—C5—C6 | 3 (2) | C32—O33—K1—O27 | -20.5 (16) |
| C4—C5—C6—C7 | -2.9 (18) | C34—O33—K1—O27 | -152.6 (12) |
| C3—C2—C7—N8 | 176.0 (10) | C32—O33—K1—O30 | -12.3 (15) |
| N1—C2—C7—N8 | -2.4 (12) | C34—O33—K1—O30 | -144.5 (13) |
| C3—C2—C7—C6 | -1.2 (17) | C32—O33—K1—O21 | 164.0 (15) |
| N1—C2—C7—C6 | -179.6 (10) | C34—O33—K1—O21 | 31.8 (13) |
| C5—C6—C7—N8 | -174.4 (12) | C32—O33—K1—O36 | 155.5 (16) |
| C5—C6—C7—C2 | 2.0 (17) | C34—O33—K1—O36 | 23.4 (12) |
| C2—C7—N8—O10 | -176.8 (10) | C32—O33—K1—O10 ⁱⁱ | -97.2 (15) |
| C6—C7—N8—O10 | 0.1 (19) | C34—O33—K1—O10 ⁱⁱ | 130.7 (12) |
| C2—C7—N8—N9 | 2.5 (12) | C32—O33—K1—Cl2 | 73.1 (16) |
| C6—C7—N8—N9 | 179.4 (11) | C34—O33—K1—Cl2 | -59.1 (12) |
| C2—N1—N9—N8 | 0.0 (12) | C32—O33—K1—C25 | -15 (2) |
| Pt1—N1—N9—N8 | -176.3 (7) | C34—O33—K1—C25 | -147.0 (17) |
| O10—N8—N9—N1 | 177.7 (9) | C32—O33—K1—C23 | 159.7 (15) |
| C7—N8—N9—N1 | -1.6 (12) | C34—O33—K1—C23 | 27.5 (17) |
| N9—N8—O10—K1 ⁱ | 147.6 (8) | C32—O33—K1—C26 | -5.1 (18) |
| C7—N8—O10—K1 ⁱ | -33.1 (15) | C34—O33—K1—C26 | -137.2 (13) |
| Cl1—Pt1—N11—N19 | 65.1 (8) | C38—O21—K1—O24 | 145.4 (10) |
| Cl2—Pt1—N11—N19 | -117.1 (8) | C22—O21—K1—O24 | 17.7 (9) |
| Cl1—Pt1—N11—C12 | -121.8 (9) | C38—O21—K1—O27 | 160.4 (9) |
| Cl2—Pt1—N11—C12 | 55.9 (9) | C22—O21—K1—O27 | 32.6 (10) |
| N19—N11—C12—C17 | 2.0 (12) | C38—O21—K1—O33 | -24.2 (10) |

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| Pt1—N11—C12—C17 | −171.5 (7) | C22—O21—K1—O33 | −151.9 (9) |
| N19—N11—C12—C13 | −178.6 (11) | C38—O21—K1—O36 | −15.6 (10) |
| Pt1—N11—C12—C13 | 7.9 (17) | C22—O21—K1—O36 | −143.4 (10) |
| C17—C12—C13—C14 | 0.7 (15) | C38—O21—K1—O10 ⁱⁱ | −133.0 (10) |
| N11—C12—C13—C14 | −178.6 (11) | C22—O21—K1—O10 ⁱⁱ | 99.2 (9) |
| C12—C13—C14—C15 | 0.3 (17) | C38—O21—K1—Cl2 | 71.6 (9) |
| C13—C14—C15—C16 | 0 (2) | C22—O21—K1—Cl2 | −56.1 (9) |
| C14—C15—C16—C17 | −0.8 (18) | C38—O21—K1—C25 | 155.4 (10) |
| N11—C12—C17—C16 | 177.6 (10) | C22—O21—K1—C25 | 27.7 (10) |
| C13—C12—C17—C16 | −1.9 (16) | C38—O21—K1—C23 | 153.4 (11) |
| N11—C12—C17—N18 | −1.2 (11) | C22—O21—K1—C23 | 25.6 (9) |
| C13—C12—C17—N18 | 179.3 (9) | C38—O21—K1—C26 | 148.5 (10) |
| C15—C16—C17—C12 | 1.9 (17) | C22—O21—K1—C26 | 20.7 (10) |
| C15—C16—C17—N18 | −179.7 (12) | C35—O36—K1—O24 | −179.6 (12) |
| C12—C17—N18—N19 | 0.0 (12) | C37—O36—K1—O24 | −40.0 (13) |
| C16—C17—N18—N19 | −178.6 (11) | C35—O36—K1—O30 | 22.2 (14) |
| C12—C17—N18—O20 | 178.1 (10) | C37—O36—K1—O30 | 161.8 (11) |
| C16—C17—N18—O20 | −1 (2) | C35—O36—K1—O33 | 10.1 (12) |
| C12—N11—N19—N18 | −2.0 (11) | C37—O36—K1—O33 | 149.7 (13) |
| Pt1—N11—N19—N18 | 172.4 (7) | C35—O36—K1—O21 | −161.0 (14) |
| O20—N18—N19—N11 | −177.0 (9) | C37—O36—K1—O21 | −21.4 (11) |
| C17—N18—N19—N11 | 1.2 (12) | C35—O36—K1—O10 ⁱⁱ | −86.3 (13) |
| C38—O21—C22—C23 | 179.7 (13) | C37—O36—K1—O10 ⁱⁱ | 53.3 (12) |
| K1—O21—C22—C23 | −49.7 (13) | C35—O36—K1—Cl2 | 109.3 (13) |
| O21—C22—C23—O24 | 66.5 (15) | C37—O36—K1—Cl2 | −111.2 (12) |
| O21—C22—C23—K1 | 35.5 (9) | C35—O36—K1—C25 | −174.4 (13) |
| C22—C23—O24—C25 | 175.4 (14) | C37—O36—K1—C25 | −34.9 (15) |
| K1—C23—O24—C25 | −136.9 (14) | C35—O36—K1—C23 | −168.3 (13) |
| C22—C23—O24—K1 | −47.7 (14) | C37—O36—K1—C23 | −28.8 (12) |
| C23—O24—C25—C26 | −177.5 (16) | C35—O36—K1—C26 | 157.2 (15) |
| K1—O24—C25—C26 | 45 (2) | C37—O36—K1—C26 | −63.3 (18) |
| C23—O24—C25—K1 | 137.9 (14) | Pt1—Cl2—K1—O24 | −172.2 (3) |
| O24—C25—C26—O27 | −64 (2) | Pt1—Cl2—K1—O27 | 126.0 (3) |
| K1—C25—C26—O27 | −33.7 (13) | Pt1—Cl2—K1—O30 | 65.8 (4) |
| O24—C25—C26—K1 | −30.0 (14) | Pt1—Cl2—K1—O33 | 5.6 (4) |
| C25—C26—O27—C28 | 179.1 (16) | Pt1—Cl2—K1—O21 | −111.6 (3) |
| K1—C26—O27—C28 | 131.0 (14) | Pt1—Cl2—K1—O36 | −53.2 (3) |
| C25—C26—O27—K1 | 48.1 (19) | Pt1—Cl2—K1—O10 ⁱⁱ | 162.9 (5) |
| C26—O27—C28—C29 | −173.2 (17) | Pt1—Cl2—K1—C25 | 167.1 (4) |
| K1—O27—C28—C29 | −43.5 (19) | Pt1—Cl2—K1—C23 | −152.7 (4) |
| O27—C28—C29—O30 | 66 (2) | Pt1—Cl2—K1—C26 | 144.5 (5) |
| C28—C29—O30—C31 | 173.9 (14) | C26—C25—K1—O24 | −139 (2) |
| C28—C29—O30—K1 | −55 (2) | C26—C25—K1—O27 | 23.8 (11) |
| C29—O30—C31—C32 | 178.5 (17) | O24—C25—K1—O27 | 162.4 (17) |
| K1—O30—C31—C32 | 46.2 (18) | C26—C25—K1—O30 | 14.2 (14) |
| O30—C31—C32—O33 | −59 (2) | O24—C25—K1—O30 | 152.8 (12) |
| C31—C32—O33—C34 | 174.4 (17) | C26—C25—K1—O33 | 16 (2) |
| C31—C32—O33—K1 | 41 (2) | O24—C25—K1—O33 | 155.1 (10) |

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| C32—O33—C34—C35 | 170.2 (18) | C26—C25—K1—O21 | −162.5 (14) |
| K1—O33—C34—C35 | −54 (2) | O24—C25—K1—O21 | −23.9 (12) |
| O33—C34—C35—O36 | 62 (2) | C26—C25—K1—O36 | −150.9 (12) |
| C34—C35—O36—C37 | 179.2 (17) | O24—C25—K1—O36 | −12.4 (17) |
| C34—C35—O36—K1 | −40 (2) | C26—C25—K1—O10 ⁱⁱ | 104.6 (13) |
| C35—O36—C37—C38 | −165.3 (16) | O24—C25—K1—O10 ⁱⁱ | −116.8 (13) |
| K1—O36—C37—C38 | 53.0 (15) | C26—C25—K1—Cl2 | −73.5 (13) |
| C22—O21—C38—C37 | 176.1 (12) | O24—C25—K1—Cl2 | 65.1 (12) |
| K1—O21—C38—C37 | 49.1 (15) | C26—C25—K1—C23 | −160.4 (17) |
| O36—C37—C38—O21 | −66.6 (17) | O24—C25—K1—C23 | −21.8 (9) |
| C23—O24—K1—O27 | −150.9 (10) | O24—C25—K1—C26 | 139 (2) |
| C25—O24—K1—O27 | −13.0 (13) | C22—C23—K1—O24 | 135.1 (14) |
| C23—O24—K1—O30 | −169.2 (9) | O24—C23—K1—O27 | 26.0 (9) |
| C25—O24—K1—O30 | −31.3 (13) | C22—C23—K1—O27 | 161.1 (9) |
| C23—O24—K1—O21 | 14.9 (9) | O24—C23—K1—O30 | 14.8 (12) |
| C25—O24—K1—O21 | 152.8 (13) | C22—C23—K1—O30 | 149.9 (8) |
| C23—O24—K1—O36 | 33.0 (10) | O24—C23—K1—O33 | −154.2 (9) |
| C25—O24—K1—O36 | 170.9 (13) | C22—C23—K1—O33 | −19.0 (15) |
| C23—O24—K1—O10 ⁱⁱ | −79.1 (9) | O24—C23—K1—O21 | −160.0 (11) |
| C25—O24—K1—O10 ⁱⁱ | 58.7 (13) | C22—C23—K1—O21 | −24.9 (8) |
| C23—O24—K1—Cl2 | 111.1 (9) | O24—C23—K1—O36 | −150.5 (9) |
| C25—O24—K1—Cl2 | −111.0 (13) | C22—C23—K1—O36 | −15.4 (9) |
| C23—O24—K1—C25 | −137.9 (17) | O24—C23—K1—O10 ⁱⁱ | 97.5 (9) |
| C25—O24—K1—C23 | 137.9 (17) | C22—C23—K1—O10 ⁱⁱ | −127.4 (9) |
| C23—O24—K1—C26 | −160.6 (12) | O24—C23—K1—Cl2 | −65.1 (9) |
| C25—O24—K1—C26 | −22.7 (13) | C22—C23—K1—Cl2 | 70.0 (8) |
| C26—O27—K1—O24 | −17.5 (12) | O24—C23—K1—C25 | 23.2 (9) |
| C28—O27—K1—O24 | −149.2 (13) | C22—C23—K1—C25 | 158.3 (12) |
| C26—O27—K1—O30 | 144.4 (13) | O24—C23—K1—C26 | 14.6 (9) |
| C28—O27—K1—O30 | 12.6 (12) | C22—C23—K1—C26 | 149.7 (10) |
| C26—O27—K1—O33 | 152.5 (12) | C25—C26—K1—O24 | 21.8 (11) |
| C28—O27—K1—O33 | 20.8 (14) | O27—C26—K1—O24 | 156.5 (16) |
| C26—O27—K1—O21 | −32.2 (13) | C25—C26—K1—O27 | −135 (2) |
| C28—O27—K1—O21 | −164.0 (12) | C25—C26—K1—O30 | −165.8 (14) |
| C26—O27—K1—O10 ⁱⁱ | −109.1 (13) | O27—C26—K1—O30 | −31.0 (12) |
| C28—O27—K1—O10 ⁱⁱ | 119.2 (13) | C25—C26—K1—O33 | −172.2 (11) |
| C26—O27—K1—Cl2 | 55.4 (13) | O27—C26—K1—O33 | −37.5 (16) |
| C28—O27—K1—Cl2 | −76.3 (13) | C25—C26—K1—O21 | 17.8 (14) |
| C26—O27—K1—C25 | −24.8 (13) | O27—C26—K1—O21 | 152.5 (12) |
| C28—O27—K1—C25 | −156.6 (15) | C25—C26—K1—O36 | 53 (2) |
| C26—O27—K1—C23 | −27.5 (13) | O27—C26—K1—O36 | −171.9 (9) |
| C28—O27—K1—C23 | −159.3 (13) | C25—C26—K1—O10 ⁱⁱ | −69.5 (13) |
| C28—O27—K1—C26 | −131.8 (18) | O27—C26—K1—O10 ⁱⁱ | 65.2 (12) |
| C29—O30—K1—O24 | 41.5 (18) | C25—C26—K1—Cl2 | 102.8 (13) |
| C31—O30—K1—O24 | 172.9 (13) | O27—C26—K1—Cl2 | −122.5 (13) |
| C29—O30—K1—O27 | 22.7 (17) | O27—C26—K1—C25 | 135 (2) |

| | | | |
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| C31—O30—K1—O27 | 154.1 (14) | C25—C26—K1—C23 | 14.1 (12) |
| C29—O30—K1—O33 | -149.2 (18) | O27—C26—K1—C23 | 148.8 (14) |

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

Hydrogen-bond geometry (\AA , $^\circ$)

| $D\text{—H}\cdots A$ | $D\text{—H}$ | $H\cdots A$ | $D\cdots A$ | $D\text{—H}\cdots A$ |
|----------------------------|--------------|-------------|-------------|----------------------|
| O20—H20…O10 ⁱⁱⁱ | 0.84 | 1.76 | 2.466 (12) | 141 |

Symmetry code: (iii) $x, -y+1/2, z-1/2$.