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(2,2′-Bipyridine-6,6′-dicarboxylato-κ^3N,N',O^6)(6′-carboxy-2,2′-bipyridine-6-carboxylato-κ^3N,N',O^6)rhodium(III)

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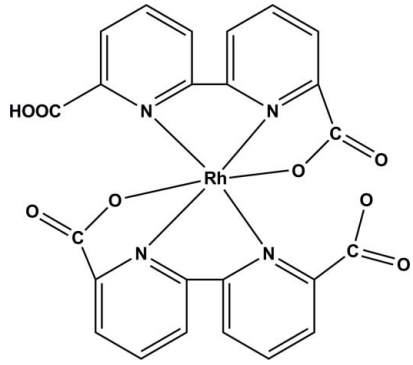
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 15.7.

The Rh^{III} ion in the title compound, $[Rh(C_{12}H_6N_2O_4)(C_{12}H_7N_2O_4)]$, is coordinated by four N atoms and two O atoms from two chelating ligands L and HL (H_2L = 2,2′-bipyridine-6,6′-dicarboxylic acid) to form a distorted octahedral geometry. Face-to-face π-stacking interactions are observed between inversion-related pyridine rings, with a centroid-to-centroid distance of 3.581 (1) Å [the perpendicular distance between the rings is 3.3980 (7) Å]. Intermolecular O—H···O hydrogen bonds link adjacent molecules into one-dimensional supramolecular chains along the c axis, while several intermolecular C—H···O interactions are also observed.



Related literature

For structures and photophysical properties of Ln^{III} (Ln is a lanthanide) complexes with the title ligand, see: Bünzli *et al.* (2000). For Rh complexes with pyridyl triazole ligands, see: Burke *et al.* (2004). For an Mn–Rh coordination polymer with the 2-methylpyrazine-5-carboxylic acid ligand, see: Chapman *et al.* (2002). For a *catena*-poly diaqua Cd^{II} complex with the title ligand, see: Knight *et al.* (2006). For a review reporting the properties of coordination polymer networks *via* O and N atoms, see: Robin & Fromm (2006). For the structures and thermal properties of five Ln complexes with the title ligand, see: Wang *et al.* (2010). For a related Ni^{II} complex with the title ligand, see: Wang *et al.* (2009).

Experimental

Crystal data

$[Rh(C_{12}H_6N_2O_4)(C_{12}H_7N_2O_4)]$
M_r = 588.29
Monoclinic, $P2_1/c$
a = 9.3308 (4) Å
b = 13.6186 (6) Å
c = 16.9974 (8) Å
β = 100.696 (1)°
V = 2122.37 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 296 K
0.2 × 0.2 × 0.2 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
15424 measured reflections
5269 independent reflections
4714 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.03
5269 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Rh1—N1	1.9529 (13)	Rh1—O5	2.0316 (13)
Rh1—N4	1.9571 (14)	Rh1—N3	2.0689 (15)
Rh1—O1	2.0226 (12)	Rh1—N2	2.0808 (14)
N2—C6—C5—N1	−2.1 (2)	N4—C15—C16—N3	−1.8 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O7^{i}	0.82	1.64	2.443 (2)	168
C2—H2···O6^{ii}	0.93	2.51	3.326 (2)	147
C4—H4A···O5^{iii}	0.93	2.54	3.341 (2)	145
C7—H7···O5^{iii}	0.93	2.51	3.304 (2)	143
C9—H9···O8^{iv}	0.93	2.36	3.097 (2)	136
C12—H12···O1^{v}	0.93	2.59	3.194 (2)	123
C17—H17···O7^{vi}	0.93	2.42	3.148 (2)	136

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); 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: ZQ2151).

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supplementary materials

Acta Cryst. (2012). E**68**, m290–m291 [doi:10.1107/S1600536812004850]

(2,2′-Bipyridine-6,6′-dicarboxylato-κ^3N,N',O^6)(6′-carboxy-2,2′-bipyridine-6-carboxylato-κ^3N,N',O^6)rhodium(III)

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Comment

Thanks to diverse coordination modes and aromatic cores, many multidentate ligands containing N- or O-donors, such as pyridine-2,6-dicarboxylic acid, 2,2′-dipyridine-4,4′-dicarboxylic acid and 2,2′-dipyridine-5,5′-dicarboxylic acid, have been widely used in metal–organic coordination chemistry (Robin & Fromm, 2006; Wang *et al.*, 2009). However, the study of complexes with the title ligand (H_2L = 2,2′-bipyridine-6,6′-dicarboxylic acid) is still rare. Some X-ray crystal structures constructed from the title ligand and metal ions, such as $[Ln_2L_3(H_2O)_3].xH_2O$ (x = 1, Ln = Eu, Tb; x = 0, Ln = Gd) (Bünzli *et al.*, 2000), $[Ln_3L_4(HL)(H_2O)_2].12H_2O$ (Ln = Ce, Nd, Pr) (Wang *et al.*, 2010), $[Ln_2L_3(H_2O)_3].3H_2O$ (Ln = Er, Tm) (Wang *et al.*, 2010), $[NiL_2].4H_2O$ (Wang *et al.*, 2009) and $[CdL]_n.2nH_2O$ (Knight *et al.*, 2006), have been investigated previously. Here we isolated a new compound constructed from the title ligand and rhodium(III) under hydrothermal conditions. A careful literature survey showed that it is the first compound constructed from rhodium(III) and the title ligand.

The structure of the title compound (Fig. 1) shows that the six-coordinated Rh^{III} atom is surrounded by four N atoms and two O atoms from the two chelated ligands to form a distorted octahedral geometry. The Rh—N bond lengths are in the range of 1.9529 (13)–2.0808 (14) Å and the Rh—O bond lengths are 2.0226 (12) and 2.0316 (13) Å (Table 1), which are comparable to other distances reported in Rh^{III} complexes (Burke *et al.*, 2004; Chapman *et al.*, 2002). The coordinated bipyridine fragments are nearly coplanar [see torsion angles of 2.1 (2) and 1.8 (2)° in Table 1].

Face-to-face π-stacking interactions between inversion-related pyridine rings with $Cg1\cdots Cg2^{ii}$ distance of 3.581 (1) Å (the perpendicular distance between the rings is 3.3980 (7) Å) are observed in the crystal structure: $Cg1$ and $Cg2$ are the centroids of the pyridine rings (N1,C1–C5) and (N2,C6–C10), respectively (symmetry code: ii = $-x$, $-y$, $-z$). A similar situation of face-to-face π-stacking interactions was observed in our early work (Wang *et al.*, 2009).

The one-dimensional chain structure of the title compound *via* hydrogen bonds is illustrated in Fig. 2. The hydrogen-bond donor O4 is connected to the acceptor O7 from the adjacent molecule to form one-dimensional infinite chains along the c-axis (O4—H4···$O7^i$ = 1.64 Å, i = x, $-y$ + 1/2, z - 1/2, Table 2). Several intermolecular C—H···O interactions contribute to stabilize the crystal structure.

Experimental

The title compound was obtained by the reaction of the mixture of $RhCl_3$ and 2,2′-dipyridine-6,6′-dicarboxylic acid in a molar ratio of 1:3 and 10 ml of water under hydrothermal conditions (at 433 K for 3 d and cooled to room temperature with a 3°C h^{-1} rate). The orange block crystals were washed with water (yield: 40%).

Refinement

The H atoms were placed in geometrically idealized positions (C—H = 0.95 Å and O—H = 0.82–0.84 Å) with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

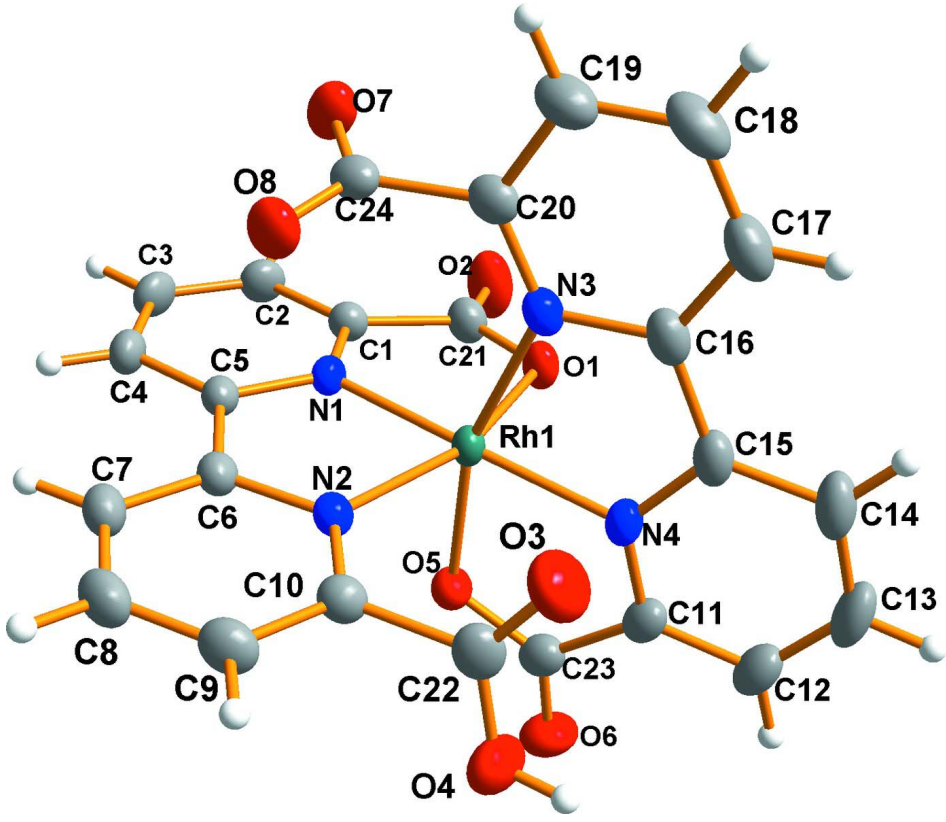

Figure 1

The structure of the title compound with 50% probability displacement ellipsoids.

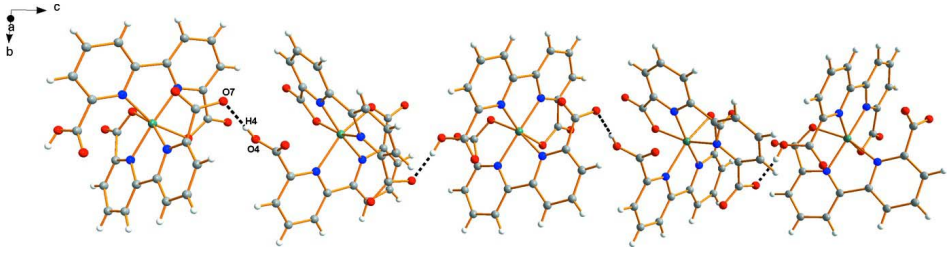

Figure 2

The one-dimensional chain structure of the title compound *via* hydrogen bonds along the *c*-axis.

(2,2′-Bipyridine-6,6′-dicarboxylato- κ^3N,N',O^6)(6′-carboxy-2,2′-bipyridine-6-carboxylato- κ^3N,N',O^6)rhodium(III)

Crystal data

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Hall symbol: -P 2ybc
$a = 9.3308$ (4) Å
$b = 13.6186$ (6) Å
$c = 16.9974$ (8) Å
$\beta = 100.696$ (1)°
$V = 2122.37$ (16) Å^3
$Z = 4$
$F(000) = 1176$
$D_x = 1.841$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.87$ mm^{-1}
$T = 296$ K
Block, orange
0.2 × 0.2 × 0.2 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
15424 measured reflections
5269 independent reflections
4714 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 12$
$k = -17 \rightarrow 18$
$l = -22 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.061$
$S = 1.03$
5269 reflections
335 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
$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 1.1072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Rh1	0.159112 (14)	0.237745 (9)	0.067212 (7)	0.02121 (5)
N1	0.08891 (15)	0.12682 (10)	0.12226 (8)	0.0225 (3)
N2	0.24130 (15)	0.12072 (10)	0.01055 (8)	0.0237 (3)
O5	−0.02277 (15)	0.23972 (9)	−0.01957 (8)	0.0298 (3)
N4	0.19640 (17)	0.35997 (10)	0.01389 (9)	0.0265 (3)

C6	0.20550 (18)	0.03125 (12)	0.03847 (10)	0.0250 (3)
C5	0.11551 (18)	0.03481 (12)	0.10163 (10)	0.0241 (3)
O1	0.05205 (14)	0.31499 (9)	0.13993 (8)	0.0287 (3)
N3	0.35387 (16)	0.27865 (11)	0.13906 (9)	0.0261 (3)
O4	0.26900 (19)	0.24099 (12)	−0.14737 (10)	0.0473 (4)
H4	0.3000	0.2889	−0.1681	0.071*
C4	0.0559 (2)	−0.04235 (13)	0.13826 (11)	0.0298 (4)
H4A	0.0739	−0.1071	0.1258	0.036*
C21	−0.0203 (2)	0.25889 (13)	0.18174 (12)	0.0297 (4)
C11	0.0918 (2)	0.38968 (13)	−0.04605 (11)	0.0299 (4)
O7	0.32750 (17)	0.11501 (10)	0.27890 (8)	0.0415 (3)
C20	0.4329 (2)	0.23263 (13)	0.20224 (11)	0.0297 (4)
O8	0.42615 (17)	0.06416 (10)	0.17725 (9)	0.0409 (3)
C24	0.3925 (2)	0.12843 (13)	0.21996 (11)	0.0299 (4)
O3	0.4556 (2)	0.26903 (12)	−0.04658 (11)	0.0534 (4)
O6	−0.13732 (17)	0.33511 (12)	−0.11836 (9)	0.0457 (4)
C1	0.00247 (19)	0.14967 (13)	0.17412 (10)	0.0257 (3)
C15	0.3070 (2)	0.41706 (13)	0.04922 (11)	0.0305 (4)
C3	−0.0313 (2)	−0.02061 (14)	0.19393 (11)	0.0330 (4)
H3	−0.0709	−0.0715	0.2195	0.040*
C7	0.2492 (2)	−0.05583 (13)	0.00854 (11)	0.0314 (4)
H7	0.2245	−0.1157	0.0287	0.038*
C9	0.3635 (2)	0.03691 (15)	−0.08131 (12)	0.0344 (4)
H9	0.4161	0.0403	−0.1227	0.041*
C16	0.3976 (2)	0.37045 (13)	0.11932 (12)	0.0308 (4)
C23	−0.0336 (2)	0.31820 (14)	−0.06556 (11)	0.0317 (4)
C8	0.3306 (2)	−0.05271 (15)	−0.05210 (12)	0.0349 (4)
H8	0.3623	−0.1104	−0.0726	0.042*
O2	−0.10279 (18)	0.29013 (11)	0.22277 (11)	0.0498 (4)
C18	0.5979 (2)	0.36721 (17)	0.22862 (14)	0.0457 (5)
H18	0.6798	0.3969	0.2588	0.055*
C2	−0.0601 (2)	0.07623 (14)	0.21197 (11)	0.0320 (4)
H2	−0.1199	0.0909	0.2485	0.038*
C13	0.2164 (3)	0.54139 (15)	−0.04621 (14)	0.0434 (5)
H13	0.2255	0.6030	−0.0684	0.052*
C10	0.31789 (19)	0.12252 (13)	−0.04881 (11)	0.0277 (3)
C14	0.3194 (2)	0.51125 (14)	0.01885 (14)	0.0399 (5)
H14	0.3949	0.5527	0.0417	0.048*
C12	0.1004 (2)	0.48196 (14)	−0.07888 (12)	0.0386 (4)
H12	0.0303	0.5034	−0.1216	0.046*
C19	0.5562 (2)	0.27527 (16)	0.24857 (14)	0.0419 (5)
H19	0.6092	0.2420	0.2922	0.050*
C22	0.3551 (2)	0.22076 (15)	−0.08135 (11)	0.0321 (4)
C17	0.5179 (2)	0.41533 (15)	0.16363 (13)	0.0400 (5)
H17	0.5452	0.4778	0.1499	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh1	0.02553 (8)	0.01557 (7)	0.02292 (7)	−0.00143 (4)	0.00549 (5)	−0.00021 (4)

N1	0.0264 (7)	0.0176 (6)	0.0235 (7)	−0.0014 (5)	0.0043 (5)	0.0010 (5)
N2	0.0262 (7)	0.0203 (6)	0.0246 (7)	−0.0007 (5)	0.0046 (6)	−0.0018 (5)
O5	0.0323 (7)	0.0257 (6)	0.0296 (7)	−0.0020 (5)	0.0010 (5)	0.0006 (5)
N4	0.0340 (8)	0.0190 (7)	0.0284 (7)	−0.0008 (6)	0.0108 (6)	0.0010 (5)
C6	0.0266 (8)	0.0215 (8)	0.0258 (8)	−0.0009 (6)	0.0021 (7)	−0.0012 (6)
C5	0.0275 (8)	0.0195 (7)	0.0240 (8)	−0.0005 (6)	0.0014 (6)	−0.0003 (6)
O1	0.0349 (7)	0.0197 (6)	0.0336 (7)	0.0008 (5)	0.0119 (5)	−0.0026 (5)
N3	0.0277 (7)	0.0221 (7)	0.0289 (7)	−0.0024 (6)	0.0063 (6)	−0.0041 (6)
O4	0.0565 (10)	0.0437 (9)	0.0410 (9)	−0.0150 (7)	0.0075 (7)	0.0115 (6)
C4	0.0366 (10)	0.0196 (8)	0.0317 (9)	−0.0019 (7)	0.0019 (7)	0.0027 (7)
C21	0.0312 (9)	0.0253 (8)	0.0332 (9)	−0.0002 (7)	0.0079 (7)	−0.0035 (7)
C11	0.0402 (10)	0.0248 (8)	0.0268 (9)	0.0052 (7)	0.0114 (7)	0.0022 (7)
O7	0.0612 (9)	0.0309 (7)	0.0357 (7)	0.0079 (7)	0.0174 (7)	0.0000 (6)
C20	0.0286 (9)	0.0299 (9)	0.0299 (9)	0.0033 (7)	0.0038 (7)	−0.0067 (7)
O8	0.0523 (9)	0.0313 (7)	0.0405 (8)	0.0085 (6)	0.0122 (7)	−0.0078 (6)
C24	0.0309 (9)	0.0282 (9)	0.0279 (9)	0.0074 (7)	−0.0017 (7)	−0.0018 (7)
O3	0.0542 (10)	0.0489 (10)	0.0556 (10)	−0.0211 (8)	0.0065 (8)	−0.0042 (8)
O6	0.0470 (9)	0.0529 (9)	0.0332 (7)	0.0040 (7)	−0.0036 (6)	0.0070 (7)
C1	0.0287 (8)	0.0245 (8)	0.0241 (8)	−0.0007 (6)	0.0054 (7)	−0.0010 (6)
C15	0.0354 (10)	0.0216 (8)	0.0375 (10)	−0.0036 (7)	0.0147 (8)	−0.0020 (7)
C3	0.0392 (10)	0.0278 (9)	0.0321 (9)	−0.0053 (7)	0.0072 (8)	0.0079 (7)
C7	0.0356 (10)	0.0226 (8)	0.0348 (10)	0.0005 (7)	0.0036 (8)	−0.0027 (7)
C9	0.0336 (10)	0.0385 (11)	0.0330 (10)	0.0039 (8)	0.0109 (8)	−0.0068 (8)
C16	0.0324 (9)	0.0247 (8)	0.0374 (10)	−0.0050 (7)	0.0116 (8)	−0.0067 (7)
C23	0.0390 (10)	0.0301 (9)	0.0266 (9)	0.0047 (8)	0.0080 (8)	−0.0009 (7)
C8	0.0359 (10)	0.0306 (10)	0.0379 (10)	0.0073 (8)	0.0057 (8)	−0.0094 (8)
O2	0.0586 (10)	0.0346 (8)	0.0667 (11)	0.0002 (7)	0.0390 (9)	−0.0092 (7)
C18	0.0322 (10)	0.0469 (13)	0.0547 (13)	−0.0081 (9)	−0.0003 (9)	−0.0187 (10)
C2	0.0367 (10)	0.0336 (9)	0.0275 (9)	−0.0027 (8)	0.0109 (7)	0.0024 (7)
C13	0.0599 (14)	0.0240 (9)	0.0528 (13)	0.0031 (9)	0.0273 (11)	0.0111 (8)
C10	0.0272 (8)	0.0289 (9)	0.0272 (8)	−0.0008 (7)	0.0054 (7)	−0.0024 (7)
C14	0.0459 (12)	0.0233 (9)	0.0554 (13)	−0.0066 (8)	0.0224 (10)	0.0000 (8)
C12	0.0537 (12)	0.0296 (10)	0.0354 (10)	0.0080 (9)	0.0159 (9)	0.0084 (8)
C19	0.0343 (10)	0.0438 (12)	0.0427 (12)	0.0021 (9)	−0.0055 (9)	−0.0096 (9)
C22	0.0350 (10)	0.0329 (10)	0.0328 (10)	−0.0022 (7)	0.0179 (8)	−0.0034 (7)
C17	0.0366 (11)	0.0323 (10)	0.0518 (12)	−0.0106 (8)	0.0101 (9)	−0.0113 (9)

Geometric parameters (Å, º)

Rh1—N1	1.9529 (13)	C20—C24	1.513 (3)
Rh1—N4	1.9571 (14)	O8—C24	1.215 (2)
Rh1—O1	2.0226 (12)	O3—C22	1.206 (3)
Rh1—O5	2.0316 (13)	O6—C23	1.213 (2)
Rh1—N3	2.0689 (15)	C1—C2	1.377 (2)
Rh1—N2	2.0808 (14)	C15—C14	1.396 (3)
N1—C5	1.337 (2)	C15—C16	1.471 (3)
N1—C1	1.337 (2)	C3—C2	1.391 (3)
N2—C10	1.341 (2)	C3—H3	0.9300
N2—C6	1.371 (2)	C7—C8	1.390 (3)
O5—C23	1.317 (2)	C7—H7	0.9300

N4—C11	1.336 (2)	C9—C8	1.374 (3)
N4—C15	1.342 (2)	C9—C10	1.390 (3)
C6—C7	1.382 (2)	C9—H9	0.9300
C6—C5	1.481 (2)	C16—C17	1.374 (3)
C5—C4	1.389 (2)	C8—H8	0.9300
O1—C21	1.313 (2)	C18—C19	1.372 (3)
N3—C20	1.340 (2)	C18—C17	1.379 (3)
N3—C16	1.376 (2)	C18—H18	0.9300
O4—C22	1.283 (3)	C2—H2	0.9300
O4—H4	0.8200	C13—C12	1.382 (3)
C4—C3	1.389 (3)	C13—C14	1.386 (3)
C4—H4A	0.9300	C13—H13	0.9300
C21—O2	1.208 (2)	C10—C22	1.513 (3)
C21—C1	1.512 (2)	C14—H14	0.9300
C11—C12	1.383 (3)	C12—H12	0.9300
C11—C23	1.511 (3)	C19—H19	0.9300
O7—C24	1.277 (2)	C17—H17	0.9300
C20—C19	1.394 (3)		

N1—Rh1—N4	169.74 (6)	N1—C1—C2	119.94 (16)
N1—Rh1—O1	82.06 (5)	N1—C1—C21	113.40 (15)
N4—Rh1—O1	89.49 (5)	C2—C1—C21	126.61 (16)
N1—Rh1—O5	92.80 (5)	N4—C15—C14	118.48 (18)
N4—Rh1—O5	81.31 (6)	N4—C15—C16	113.04 (15)
O1—Rh1—O5	89.77 (5)	C14—C15—C16	128.44 (18)
N1—Rh1—N3	105.16 (6)	C4—C3—C2	120.91 (17)
N4—Rh1—N3	80.34 (6)	C4—C3—H3	119.5
O1—Rh1—N3	88.77 (5)	C2—C3—H3	119.5
O5—Rh1—N3	161.60 (5)	C6—C7—C8	119.09 (18)
N1—Rh1—N2	79.31 (6)	C6—C7—H7	120.5
N4—Rh1—N2	108.94 (6)	C8—C7—H7	120.5
O1—Rh1—N2	161.35 (5)	C8—C9—C10	119.73 (18)
O5—Rh1—N2	90.23 (5)	C8—C9—H9	120.1
N3—Rh1—N2	96.93 (6)	C10—C9—H9	120.1
C5—N1—C1	123.71 (15)	C17—C16—N3	121.32 (19)
C5—N1—Rh1	120.29 (12)	C17—C16—C15	122.71 (17)
C1—N1—Rh1	115.65 (11)	N3—C16—C15	115.96 (16)
C10—N2—C6	118.36 (15)	O6—C23—O5	123.79 (19)
C10—N2—Rh1	128.91 (12)	O6—C23—C11	121.25 (18)
C6—N2—Rh1	112.71 (11)	O5—C23—C11	114.92 (16)
C23—O5—Rh1	113.81 (12)	C9—C8—C7	119.00 (17)
C11—N4—C15	123.93 (15)	C9—C8—H8	120.5
C11—N4—Rh1	116.31 (12)	C7—C8—H8	120.5
C15—N4—Rh1	118.27 (12)	C19—C18—C17	119.67 (19)
N2—C6—C7	121.85 (16)	C19—C18—H18	120.2
N2—C6—C5	115.40 (14)	C17—C18—H18	120.2
C7—C6—C5	122.74 (15)	C1—C2—C3	118.00 (17)
N1—C5—C4	118.83 (16)	C1—C2—H2	121.0
N1—C5—C6	112.24 (14)	C3—C2—H2	121.0

C4—C5—C6	128.90 (15)	C12—C13—C14	121.48 (18)
C21—O1—Rh1	112.97 (10)	C12—C13—H13	119.3
C20—N3—C16	118.43 (16)	C14—C13—H13	119.3
C20—N3—Rh1	129.77 (12)	N2—C10—C9	121.95 (17)
C16—N3—Rh1	111.63 (12)	N2—C10—C22	118.83 (16)
C22—O4—H4	109.5	C9—C10—C22	119.23 (16)
C5—C4—C3	118.54 (16)	C13—C14—C15	118.33 (19)
C5—C4—H4A	120.7	C13—C14—H14	120.8
C3—C4—H4A	120.7	C15—C14—H14	120.8
O2—C21—O1	123.68 (17)	C13—C12—C11	118.02 (19)
O2—C21—C1	120.73 (17)	C13—C12—H12	121.0
O1—C21—C1	115.58 (15)	C11—C12—H12	121.0
N4—C11—C12	119.57 (18)	C18—C19—C20	118.9 (2)
N4—C11—C23	113.49 (15)	C18—C19—H19	120.6
C12—C11—C23	126.69 (18)	C20—C19—H19	120.6
N3—C20—C19	122.11 (18)	O3—C22—O4	128.0 (2)
N3—C20—C24	118.53 (16)	O3—C22—C10	120.88 (19)
C19—C20—C24	119.22 (18)	O4—C22—C10	111.14 (16)
O8—C24—O7	125.35 (18)	C16—C17—C18	119.59 (19)
O8—C24—C20	117.09 (17)	C16—C17—H17	120.2
O7—C24—C20	117.56 (16)	C18—C17—H17	120.2

N4—Rh1—N1—C5	142.4 (3)	Rh1—N4—C11—C12	170.67 (14)
O1—Rh1—N1—C5	177.26 (13)	C15—N4—C11—C23	−169.87 (16)
O5—Rh1—N1—C5	87.88 (13)	Rh1—N4—C11—C23	−4.10 (19)
N3—Rh1—N1—C5	−96.19 (13)	C16—N3—C20—C19	0.7 (3)
N2—Rh1—N1—C5	−1.83 (12)	Rh1—N3—C20—C19	−174.12 (15)
N4—Rh1—N1—C1	−31.0 (4)	C16—N3—C20—C24	−174.99 (16)
O1—Rh1—N1—C1	3.86 (12)	Rh1—N3—C20—C24	10.2 (2)
O5—Rh1—N1—C1	−85.52 (12)	N3—C20—C24—O8	75.6 (2)
N3—Rh1—N1—C1	90.41 (13)	C19—C20—C24—O8	−100.2 (2)
N2—Rh1—N1—C1	−175.23 (13)	N3—C20—C24—O7	−105.1 (2)
N1—Rh1—N2—C10	178.45 (16)	C19—C20—C24—O7	79.0 (2)
N4—Rh1—N2—C10	4.76 (16)	C5—N1—C1—C2	2.6 (3)
O1—Rh1—N2—C10	175.62 (15)	Rh1—N1—C1—C2	175.79 (13)
O5—Rh1—N2—C10	85.64 (15)	C5—N1—C1—C21	−174.92 (15)
N3—Rh1—N2—C10	−77.37 (15)	Rh1—N1—C1—C21	−1.77 (19)
N1—Rh1—N2—C6	0.49 (11)	O2—C21—C1—N1	175.54 (19)
N4—Rh1—N2—C6	−173.19 (11)	O1—C21—C1—N1	−3.0 (2)
O1—Rh1—N2—C6	−2.3 (2)	O2—C21—C1—C2	−1.8 (3)
O5—Rh1—N2—C6	−92.31 (12)	O1—C21—C1—C2	179.66 (17)
N3—Rh1—N2—C6	104.68 (12)	C11—N4—C15—C14	−4.0 (3)
N1—Rh1—O5—C23	168.90 (13)	Rh1—N4—C15—C14	−169.55 (14)
N4—Rh1—O5—C23	−2.66 (12)	C11—N4—C15—C16	173.52 (16)
O1—Rh1—O5—C23	86.86 (12)	Rh1—N4—C15—C16	8.0 (2)
N3—Rh1—O5—C23	1.4 (2)	C5—C4—C3—C2	0.9 (3)
N2—Rh1—O5—C23	−111.79 (13)	N2—C6—C7—C8	−0.6 (3)
N1—Rh1—N4—C11	−51.6 (4)	C5—C6—C7—C8	178.45 (16)
O1—Rh1—N4—C11	−86.07 (13)	C20—N3—C16—C17	−1.0 (3)

O5—Rh1—N4—C11	3.78 (12)	Rh1—N3—C16—C17	174.67 (15)
N3—Rh1—N4—C11	−174.92 (13)	C20—N3—C16—C15	179.72 (16)
N2—Rh1—N4—C11	91.02 (13)	Rh1—N3—C16—C15	−4.57 (19)
N1—Rh1—N4—C15	115.0 (3)	N4—C15—C16—C17	178.97 (17)
O1—Rh1—N4—C15	80.54 (13)	C14—C15—C16—C17	−3.8 (3)
O5—Rh1—N4—C15	170.39 (14)	N4—C15—C16—N3	−1.8 (2)
N3—Rh1—N4—C15	−8.30 (13)	C14—C15—C16—N3	175.46 (18)
N2—Rh1—N4—C15	−102.37 (13)	Rh1—O5—C23—O6	−176.56 (16)
C10—N2—C6—C7	1.6 (2)	Rh1—O5—C23—C11	1.25 (19)
Rh1—N2—C6—C7	179.84 (14)	N4—C11—C23—O6	179.66 (17)
C10—N2—C6—C5	−177.49 (15)	C12—C11—C23—O6	5.3 (3)
Rh1—N2—C6—C5	0.70 (18)	N4—C11—C23—O5	1.8 (2)
C1—N1—C5—C4	−2.9 (3)	C12—C11—C23—O5	−172.54 (18)
Rh1—N1—C5—C4	−175.79 (12)	C10—C9—C8—C7	1.4 (3)
C1—N1—C5—C6	175.50 (15)	C6—C7—C8—C9	−0.9 (3)
Rh1—N1—C5—C6	2.7 (2)	N1—C1—C2—C3	−0.5 (3)
N2—C6—C5—N1	−2.1 (2)	C21—C1—C2—C3	176.71 (18)
C7—C6—C5—N1	178.79 (16)	C4—C3—C2—C1	−1.2 (3)
N2—C6—C5—C4	176.16 (17)	C6—N2—C10—C9	−1.2 (3)
C7—C6—C5—C4	−3.0 (3)	Rh1—N2—C10—C9	−179.03 (13)
N1—Rh1—O1—C21	−5.47 (13)	C6—N2—C10—C22	178.66 (15)
N4—Rh1—O1—C21	168.69 (13)	Rh1—N2—C10—C22	0.8 (2)
O5—Rh1—O1—C21	87.39 (13)	C8—C9—C10—N2	−0.3 (3)
N3—Rh1—O1—C21	−110.96 (13)	C8—C9—C10—C22	179.85 (18)
N2—Rh1—O1—C21	−2.7 (2)	C12—C13—C14—C15	2.5 (3)
N1—Rh1—N3—C20	10.65 (17)	N4—C15—C14—C13	0.3 (3)
N4—Rh1—N3—C20	−178.22 (16)	C16—C15—C14—C13	−176.87 (19)
O1—Rh1—N3—C20	92.09 (16)	C14—C13—C12—C11	−1.7 (3)
O5—Rh1—N3—C20	177.68 (16)	N4—C11—C12—C13	−1.9 (3)
N2—Rh1—N3—C20	−70.10 (16)	C23—C11—C12—C13	172.14 (18)
N1—Rh1—N3—C16	−164.44 (12)	C17—C18—C19—C20	0.0 (3)
N4—Rh1—N3—C16	6.69 (12)	N3—C20—C19—C18	−0.2 (3)
O1—Rh1—N3—C16	−83.00 (12)	C24—C20—C19—C18	175.48 (19)
O5—Rh1—N3—C16	2.6 (2)	N2—C10—C22—O3	79.9 (2)
N2—Rh1—N3—C16	114.81 (12)	C9—C10—C22—O3	−100.3 (2)
N1—C5—C4—C3	1.1 (3)	N2—C10—C22—O4	−100.8 (2)
C6—C5—C4—C3	−177.02 (17)	C9—C10—C22—O4	79.0 (2)
Rh1—O1—C21—O2	−172.48 (18)	N3—C16—C17—C18	0.9 (3)
Rh1—O1—C21—C1	6.0 (2)	C15—C16—C17—C18	−179.95 (19)
C15—N4—C11—C12	4.9 (3)	C19—C18—C17—C16	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O7^{i}	0.82	1.64	2.443 (2)	168
C2—H2···O6^{ii}	0.93	2.51	3.326 (2)	147
C4—H4*A*···O5^{iii}	0.93	2.54	3.341 (2)	145
C7—H7···O5^{iii}	0.93	2.51	3.304 (2)	143
C9—H9···O8^{iv}	0.93	2.36	3.097 (2)	136

C12—H12···O1^{v}	0.93	2.59	3.194 (2)	123
C17—H17···O7^{vi}	0.93	2.42	3.148 (2)	136

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