

C24	0.6775 (7)	0.2075 (6)	0.4030 (3)	0.076 (5)
C25	0.6597 (7)	0.1285 (6)	0.4331 (2)	0.077 (5)
C26	0.6432 (6)	0.0150 (6)	0.4232 (2)	0.062 (4)
C27	0.5829 (5)	-0.2399 (5)	0.4069 (2)	0.052 (3)
C28	0.4638 (6)	-0.2119 (6)	0.4242 (2)	0.062 (4)
C29	0.4004 (7)	-0.2820 (7)	0.4514 (2)	0.074 (4)
C30	0.4524 (8)	-0.3874 (7)	0.4599 (2)	0.081 (5)
C31	0.5665 (9)	-0.4202 (7)	0.4426 (2)	0.083 (5)
C32	0.6316 (8)	-0.3475 (6)	0.4171 (2)	0.073 (5)
C33	0.5646 (5)	-0.1946 (4)	0.3294 (1)	0.042 (3)
C34	0.4535 (5)	-0.1341 (5)	0.3129 (2)	0.057 (4)
C35	0.3762 (6)	-0.1688 (6)	0.2778 (2)	0.068 (4)
C36	0.4085 (7)	-0.2664 (7)	0.2588 (2)	0.073 (4)
C37	0.5159 (6)	-0.3300 (6)	0.2736 (2)	0.059 (4)
C38	0.5922 (6)	-0.2950 (5)	0.3087 (2)	0.051 (3)
C39	0.8171 (5)	-0.1808 (4)	0.3708 (2)	0.047 (3)
C40	0.9018 (6)	-0.1801 (5)	0.4068 (2)	0.065 (4)
C41	1.0454 (7)	-0.1811 (6)	0.4060 (3)	0.076 (5)
C42	1.1054 (7)	-0.1840 (5)	0.3699 (3)	0.070 (4)
C43	1.0258 (6)	-0.1850 (5)	0.3337 (2)	0.061 (4)
C44	0.8844 (5)	-0.1836 (5)	0.3351 (2)	0.049 (3)
B	0.6503 (6)	-0.1606 (5)	0.3726 (2)	0.046 (3)
Cl2	0.0878 (5)	-0.4060 (5)	0.5003 (1)	0.258 (5)
C51†	-0.060 (2)	-0.441 (2)	0.4880 (5)	0.12 (1)

† Disordered atom; site occupancy = 0.5.

Table 2. Selected geometric parameters (Å, °)

Ru—Cl1	2.389 (2)	Ru—C13	2.198 (5)
Ru—S	2.358 (2)	Ru—C14	2.245 (5)
Ru—P	2.312 (2)	Ru—C15	2.267 (6)
Ru—C11	2.212 (5)	Ru—C16	2.246 (5)
Ru—C12	2.198 (5)		
Cl1—Ru—S	90.81 (6)	S—Ru—P	83.86 (6)
Cl1—Ru—P	85.63 (6)	S—Ru—C11	162.6 (1)
Cl1—Ru—C13	156.6 (1)	P—Ru—C15	162.7 (1)

The C51 atom of the CH₂Cl₂ solvate molecule has a site-occupation factor of 0.5. All H atoms were included in the structural refinement, except for those of the CH₂Cl₂ solvate molecule. The structure solution and refinement used *Xtal3.2* (Hall, Flack & Stewart, 1992).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1989). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *Xtal3.2 DIFDAT ABSORB ADDREF SORTRF*. Molecular graphics: *Xtal3.2*. Software used to prepare material for publication: *Xtal3.2*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1286). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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cis-Diaquabis(2,2'-bipyrimidine-*N,N'*)-cobalt(II) Diperchlorate Dihydrate, [Co(C₈H₆N₄)₂(H₂O)₂](ClO₄)₂.2H₂O

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Abstract

The complex cation in the title structure has a distorted octahedral coordination geometry with cobalt bonded to two bidentate bipyrimidine (bpm) ligands and two water molecules in *cis* positions. The structure has crystallographically imposed twofold symmetry.

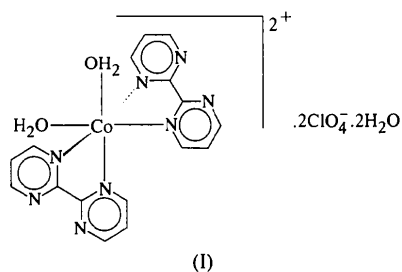
Comment

Our interest in complexes of bipyridine-type ligands stems from studies of their diffusion behavior in clays. In our case, diffusion properties are measured electrochemically using prepared clay electrodes (Lee & Fitch, 1990). Earlier, an anomalous diffusion behavior was noted for [Cr(bipy)₃]³⁺ (bipy is bipyridine; Edens, Fitch & Lavy-Feder, 1991) and this led to the preparation and testing of complexes with similar ligands.

The ligand 2,2'-bipyrimidine (bpm) has four N donor atoms so it can coordinate as a bidentate ligand to a single metal atom or as a bis-bidentate bridging

ligand connecting two metal atoms. The dinuclear compound μ -bpm-bis[Co(bpm)(SCN)₂] is an example that incorporates both types of coordination (De Munno, Julve, Lloret, Faus & Caneschi, 1994). For our purposes, when only one pair of bpm donor atoms is coordinated to a metal atom, then the second pair may interact with a clay surface, thus possibly influencing the mobility of metal complexes in clays and altering diffusion rates. We therefore prepared and tested a range of bpm complexes.

The main feature of the title complex, (I), is the distorted octahedral complex cation composed of cobalt bonded to two bidentate bpm ligands and two water molecules in *cis* positions. The site symmetry of the Co atom imposes twofold symmetry on the complex and structure. The twofold axis bisects the O5—Co—O5' bond angle [symmetry code: (i) $-x, y, \frac{1}{2} - z$].



In the complex cation of (I), the distance between coordinated N atoms is 2.651 (2) Å, whereas that between uncoordinated N atoms is 2.738 (3) Å (Fig. 1). Comparable distances in the free ligand are all equal to 2.711 Å (Fernholt, Romming & Samdal, 1981). This results in an in-plane bending of the ligand towards the metal atom and an associated bite angle of 77.18 (7)°. The torsion angle of the chelate ring (N1—C4—C5—N3) is essentially zero [0.0(3)°], while the dihedral angle between the linked six-membered rings is 4.68 (13)°.

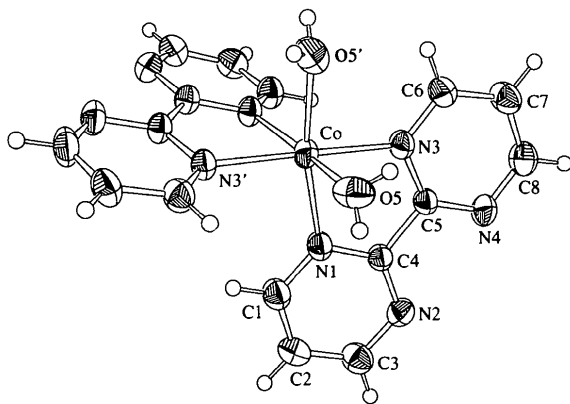


Fig. 1. An ORTEPII diagram (Johnson, 1976) of [Co(bpm)₂(H₂O)₂]²⁺ showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

The perchlorate anion was found to be rotationally disordered. It is represented as two partially occupied tetrahedra sharing a common bond. Consequently, two sets of O2, O3 and O4 atoms are reported and labeled as *A* and *B*. A solvent water molecule is also present. All water H atoms were located and refined. Final H—O distances range from 0.71 (2) to 0.83 (2) Å and the H—O—H angles were 104 (4) and 108 (4)°.

The crystal is constructed of layers of perchlorate anions alternating with layers containing coordination cations and solvent molecules. The layers are perpendicular to the *a* axis (Fig. 2).

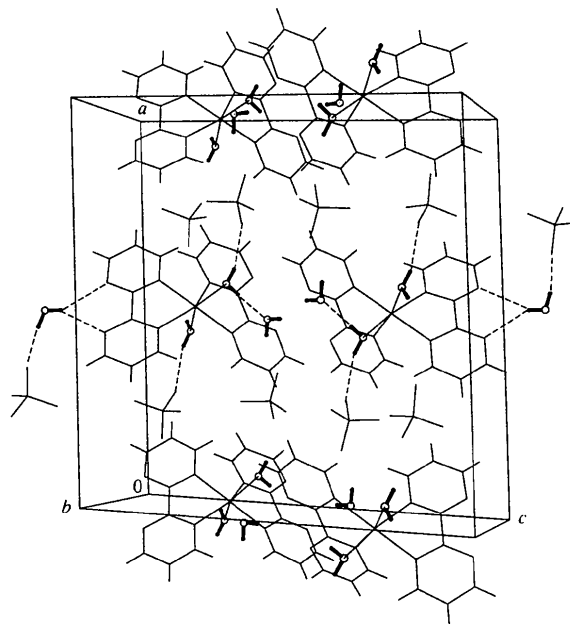


Fig. 2. An ORTEPII (Johnson, 1976) diagram of the unit cell of (I) showing the packing and selected hydrogen bonds. Water molecules are depicted with wider solid bonds and larger arbitrary radii. Hydrogen bonds from solvent water are only shown at the left and right extremes of the cell outline, and hydrogen bonds from coordinated water are only shown inside the cell outline. The perchlorate anion shown has the larger occupancy factor of the disordered pair.

There is an extensive network of hydrogen bonding within and between the layers (Fig. 2). Coordinated water molecules donate a single hydrogen bond both to the solvent [H5A···O6ⁱⁱ 1.91 (3) Å and 174 (4)°] and a perchlorate O atom [H5B···O2Aⁱ 2.13 (3) Å and 161 (4)°; H5B···O2Bⁱ 2.13 (3) Å and 137 (3)°]. In each pair of values, the first refers to the H···A distance (Å) and the second to the O—H···A angle (°); symmetry operations are as given in Table 3. Solvent water donates a single hydrogen bond to a perchlorate O atom [H6A···O3Aⁱⁱⁱ 2.19 (3) Å and

162 (3)°; H6A···O4Bⁱⁱⁱ 2.26 (3) Å and 156 (3)°] and also forms a bifurcated hydrogen bond to uncoordinated N atoms [H6B···N2^{iv} 2.57 (3) Å and 145 (4)°; H6B···N4^{iv} 2.43 (3) and 147 (4)°]. These bifurcated links run parallel to the *c* axis. Hydrogen bonds to uncoordinated N atoms are quite weak and if this is also the case in solution, then their interaction with a clay surface may be possible.

A search for bpm-containing compounds in the Cambridge Structural Database (Allen *et al.*, 1987) showed over 50 entries, most of which are multinuclear metal complexes. The structure most similar to the title compound is that of *cis*-[Co(bpm)₂Cl₂] (De Munno, Nicolo & Julve, 1993). In this compound, the bpm ligands and chloride anions are crystallographically independent. The two ligands have smaller 'bite' angles of 75.4 (1) and 75.8 (1)°, larger chelate ring torsion angles of 5.10 and 10.41°, and larger dihedral angles of 8.8 (1) and 12.5 (1)° for linked-pairs of six-membered rings. All Co—N bond distances are significantly longer in the dichloro complex and the Cl—Co—Cl' angle is 100.7 (1)°, the N1—Co—N1' angle 82.3 (1)° and the N3—Co—N3' angle 169.9 (1)°. Comparable angles in the diaqua complex are 82.4 (1), 95.8 (1) and 177.3 (1)°, respectively. Clearly the larger size of the Cl atom results in a more distorted complex.

Experimental

The title compound was prepared by Yunlong Wang by the dropwise addition of a solution of bpm (4.4 mmol) in methanol (10 ml) to a solution of CoCl₂·6H₂O (2.0 mmol) in methanol (20 ml), while stirring the receiving solution at 308 K. All manipulations were carried out under an N₂ atmosphere. A red precipitate formed. Addition of HClO₄ (1.0 ml) in H₂O₂ (1.0 ml) caused conversion to a yellow solid after several hours. Recrystallization from water afforded yellow crystals of the title compound.

Crystal data

[Co(C₈H₆N₄)₂(H₂O)₂]-
(ClO₄)₂·2H₂O

M_r = 646.24

Monoclinic

*C*2/*c*

a = 18.104 (3) Å

b = 7.6912 (11) Å

c = 17.600 (3) Å

β = 93.687 (7)°

V = 2445.6 (6) Å³

Z = 4

D_x = 1.755 Mg m⁻³

D_m = 1.75 (1) Mg m⁻³

D_m measured by flotation in
an aqueous ZnCl₂ solution

Data collection

Picker FACS-I diffractometer

Mo *K*α radiation

λ = 0.7107 Å

Cell parameters from 18
reflections

θ = 10.1–13.6°

μ = 0.999 mm⁻¹

T = 295 (2) K

Irregular cut block

0.56 × 0.53 × 0.50 mm

Yellow

R_{int} = 0.022

θ_{max} = 26.5°

θ/2θ scans

Absorption correction:

ψ scan (Pavkovic,

Wilhelm & Brown, 1978)

T_{min} = 0.57, *T_{max}* = 0.61

6282 measured reflections

2543 independent reflections

2206 observed reflections

[*I* > 2σ(*I*)]

Refinement

Refinement on *F*²

R(*F*) = 0.034

w*R*(*F*²) = 0.102

S = 1.060

2543 reflections

244 parameters

w = 1/[σ²(*F_o*²) + (0.0535*P*)²
+ 1.281*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.32 e Å⁻³

Δρ_{min} = -0.41 e Å⁻³

h = -22 → 21

k = -3 → 9

l = -22 → 21

3 standard reflections
monitored every 150
reflections

intensity decay: 4%

Extinction correction:

SHELXL93 (Sheldrick,
1993)

Extinction coefficient:

0.0002 (3)

Atomic scattering factors

from *International Tables
for Crystallography* (1992,
Vol. C, Tables 4.2.6.8 and
6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i>
Co	0	0.08286 (5)	1/4	0.0308 (2)
Cl	0.26408 (3)	0.01254 (8)	0.35975 (3)	0.0403 (2)
O1	0.24095 (13)	0.1155 (3)	0.42067 (12)	0.0672 (6)
O2A†	0.2159 (2)	-0.1326 (6)	0.3475 (4)	0.089 (2)
O3A	0.3375 (2)	-0.0468 (6)	0.3743 (2)	0.0599 (13)
O4A	0.2610 (4)	0.1153 (7)	0.2926 (2)	0.098 (2)
O2B	0.2078 (6)	-0.031 (3)	0.3092 (6)	0.107 (5)
O3B	0.2993 (15)	-0.1330 (18)	0.3902 (9)	0.204 (13)
O4B	0.3167 (7)	0.1121 (16)	0.3223 (7)	0.096 (5)
O5	-0.06147 (10)	-0.1231 (3)	0.19878 (11)	0.0493 (4)
O6	0.02316 (11)	0.6620 (3)	0.11984 (10)	0.0498 (4)
N1	-0.05753 (9)	0.2678 (2)	0.17916 (9)	0.0333 (4)
N2	-0.07176 (10)	0.3580 (3)	0.05057 (10)	0.0376 (4)
N3	0.06332 (9)	0.0894 (2)	0.15212 (10)	0.0320 (4)
N4	0.05268 (10)	0.1729 (3)	0.02222 (10)	0.0407 (4)
C1	-0.11452 (13)	0.3677 (3)	0.19585 (13)	0.0400 (5)
C2	-0.15115 (12)	0.4695 (3)	0.14136 (15)	0.0433 (5)
C3	-0.12877 (13)	0.4568 (3)	0.06840 (14)	0.0437 (5)
C4	-0.03740 (11)	0.2722 (3)	0.10718 (11)	0.0307 (4)
C5	0.03031 (11)	0.1722 (3)	0.09239 (11)	0.0305 (4)
C6	0.12472 (12)	-0.0008 (3)	0.14010 (14)	0.0392 (5)
C7	0.15204 (13)	-0.0092 (3)	0.06890 (14)	0.0434 (6)
C8	0.11387 (14)	0.0804 (4)	0.01179 (14)	0.0464 (6)

† Atoms labeled A and B have site-occupancy factors of 0.702 (10) and 0.298 (10), respectively.

Table 2. Selected geometric parameters (Å, °)

Co—O5	2.105 (2)	N3—C6	1.339 (3)
Co—N1	2.120 (2)	N4—C5	1.324 (3)
Co—N3	2.130 (2)	N4—C8	1.339 (3)
N1—C1	1.335 (3)	C1—C2	1.375 (3)
N1—C4	1.341 (3)	C2—C3	1.375 (4)
N2—C4	1.317 (3)	C4—C5	1.484 (3)
N2—C3	1.335 (3)	C6—C7	1.378 (3)
N3—C5	1.337 (3)	C7—C8	1.369 (4)
O5—Co—O5 ⁱ	82.38 (11)	C6—N3—Co	127.7 (2)
O5—Co—N1 ⁱ	169.36 (7)	C5—N4—C8	115.5 (2)
O5 ⁱ —Co—N1 ⁱ	91.53 (8)	N1—C1—C2	121.3 (2)
N1 ⁱ —Co—N1	95.75 (10)	C3—C2—C1	117.0 (2)

O5—Co—N3'	93.84 (7)	N2—C3—C2	122.6 (2)
O5' ⁱ —Co—N3'	88.20 (7)	N2—C4—N1	125.7 (2)
N1' ⁱ —Co—N3'	77.18 (7)	N2—C4—C5	118.8 (2)
N1—Co—N3'	100.96 (6)	N1—C4—C5	115.5 (2)
N3' ⁱ —Co—N3	177.29 (10)	N4—C5—N3	126.0 (2)
C1—N1—C4	117.0 (2)	N4—C5—C4	117.8 (2)
C1—N1—Co	127.91 (14)	N3—C5—C4	116.2 (2)
C4—N1—Co	114.82 (14)	N3—C6—C7	121.2 (2)
C4—N2—C3	116.2 (2)	C8—C7—C6	116.8 (2)
C5—N3—C6	117.2 (2)	N4—C8—C7	123.4 (2)
C5—N3—Co	114.24 (13)		

Symmetry code: (i) $-x, y, \frac{1}{2} - z$.

Table 3. Hydrogen-bonding geometry (Å, °)

D—H...A	D—H	H...A	D—H...A
O5—H5A...O6 ⁱ	0.79 (3)	1.91 (3)	174 (4)
O5—H5B...O2A ⁱⁱ	0.77 (3)	2.13 (3)	161 (4)
O5—H5B...O2B ⁱⁱ	0.77 (3)	2.13 (3)	137 (3)
O6—H6A...O3A ⁱⁱⁱ	0.83 (3)	2.19 (3)	162 (3)
O6—H6A...O4B ⁱⁱⁱ	0.83 (3)	2.26 (3)	156 (3)
O6—H6B...N2 ^{iv}	0.71 (3)	2.57 (3)	145 (4)
O6—H6B...N4 ^{iv}	0.71 (3)	2.43 (3)	147 (4)

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

Several restraints were imposed on the model structure during refinement. The perchlorate anion is rotationally disordered about the O1—C1 bond. This feature was modeled as two tetrahedra (A and B) having a common O1—C1 bond, restrained to have a net occupancy of 1. Final occupancy factors for the A and B sets of O2, O3 and O4 atoms are 0.71 (1) and 0.29 (1), respectively. The disordered anion was also restrained to have tetrahedral geometry by fixing the C1—O and O—O distances (20 restraints). Refinement of the four water H atoms was subject to a common H—O distance and displacement parameter (six restraints). The final distance parameter was 0.78 (2) Å and the displacement parameter was 0.071 (5) Å². H atoms bonded to C atoms were placed in calculated positions using a riding model with a fixed C—H distance of 0.93 Å. They were assigned isotropic displacement parameters of 1.2 times that of the parent C atom. The 244 parameters varied in the refinement included an extinction parameter and an overall scale factor. The largest peaks in the final electron-density difference map were associated with the disordered O atoms.

Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1247). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). **C52**, 2987–2989

[2,2'-Oxybis(1,1,1,3,3,3-hexafluoro-2-propanolato-O)](N,N,N',N'-tetramethylethylenediamine-N,N')copper(II) Hemibenzene Solvate

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Abstract

The title compound, [Cu(C₆F₁₂O₃)(C₆H₁₆N₂)]·0.5C₆H₆, forms a four-coordinate complex, with the Cu^{II} ion in a slightly distorted square-planar environment. The six-membered chelate ring and the co-ligand form a complex with approximate molecular C₂ symmetry. The benzene solvate molecule lies on a crystallographic inversion center.

Comment

Fluorinated *gem*-diols have been observed as an [O—C(CF₃)₂—O]²⁻ dialkoxide, forming a four-membered chelate ring with the transition metal ions Cu^{II} and Ni^{II} (Bradford, Hynes, Payne & Willis, 1990), and Pt^{II} (Hynes, Willis & Payne, 1992). The condensed dialkoxide [O—C(CF₃)₂—O—C(CF₃)₂—O]²⁻ has been shown to form a six-membered ring with Pt^{II} (Modinos & Woodward, 1975). In the title complex, [(Me₂NCH₂—CH₂NMe₂)Cu{OC(CF₃)₂OC(CF₃)₂O}].0.5C₆H₆, (I), the dialkoxide forms a six-membered ring with the four-coordinate Cu^{II} ion, in a complex with a N,N,N',N'-tetramethylethylenediamine (TMEDA) co-ligand. A benzene solvate molecule is also present in an asymmet-