

Bis(2-amino-4-methylpyrimidin-3-ium) *trans*-diaquabis(pyrazine-2,3-dicarboxylato)cobaltate(II) hexahydrate

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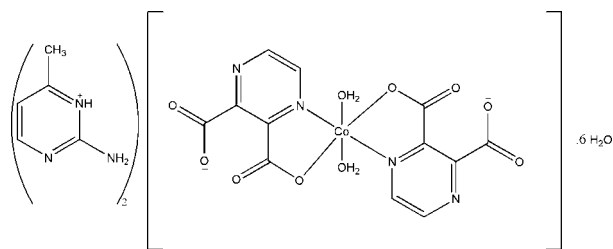
Received 30 August 2010; accepted 21 September 2010

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.025; wR factor = 0.064; data-to-parameter ratio = 10.8.

In the crystal structure of the mononuclear title compound, $(\text{C}_5\text{H}_8\text{N}_3)_2[\text{Co}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 6\text{H}_2\text{O}$ or $(\text{ampymH})_2[\text{Co}(\text{pyzdc})_2(\text{H}_2\text{O})_2] \cdot 6\text{H}_2\text{O}$ (ampym = 2-amino-4-methyl pyrimidine, pyzdcH_2 = pyrazine-2,3-dicarboxylic acid), the Co^{II} ion is hexacoordinated by two $(\text{pyzdc})^{2-}$ groups in the equatorial plane and two water molecules in axial positions, giving an N_2CoO_4 bound set. The $(\text{pyzdc})^{2-}$ anion acts as a bidentate ligand through one carboxylate group O atom and pyrazine ring N atom. There are diverse $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen-bonding interactions, which lead to the formation of a three-dimensional supramolecular architecture. Off-set or slipped $\pi-\pi$ stacking interactions are also observed between adjacent pyrimidine rings with face-to-face distances of 3.6337 (9) Å.

Related literature

For the pyzdcH_2 ligand, see: Aghabozorg *et al.* (2008). For the crystal structure of pyrazine-2,3-dicarboxylic acid (pyzdcH_2), see: Takusagawa & Shimada (1973). For complexes of pyzdcH_2 with zinc and manganese, see: Eshtiagh-Hosseini *et al.* (2010*a,b,c,d,e*). The six uncoordinated water molecules increase the number of hydrogen bonds and lead to the formation of $(\text{H}_2\text{O})_n$ clusters throughout the crystal, see: Aghabozorg *et al.* (2010).



Experimental

Crystal data

$(\text{C}_5\text{H}_8\text{N}_3)_2[\text{Co}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)_2 \cdot (\text{H}_2\text{O})_2] \cdot 6\text{H}_2\text{O}$
 $M_r = 755.54$
Triclinic, $P\bar{1}$
 $a = 6.5880$ (4) Å
 $b = 8.0591$ (5) Å
 $c = 15.0285$ (8) Å
 $\alpha = 98.085$ (5)°

$\beta = 96.940$ (4)°
 $\gamma = 91.261$ (5)°
 $V = 783.58$ (8) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 0.64$ mm⁻¹
 $T = 120$ K
0.40 × 0.40 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire2 detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford

Diffraction, 2009)
 $T_{\text{min}} = 0.903$, $T_{\text{max}} = 1.000$
5733 measured reflections
2758 independent reflections
2428 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.011$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.064$
 $S = 1.04$
2758 reflections
256 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.30$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N3}-\text{H3A} \cdots \text{O3}^{\text{i}}$	0.88	1.77	2.6487 (17)	172
$\text{N5}-\text{H5C} \cdots \text{O21}^{\text{ii}}$	0.88	1.96	2.8350 (18)	172
$\text{N5}-\text{H5D} \cdots \text{O4}^{\text{i}}$	0.88	1.96	2.8310 (18)	171
$\text{O21}-\text{H21B} \cdots \text{O4}^{\text{iii}}$	0.81 (2)	1.97 (3)	2.7777 (18)	175 (2)
$\text{O21}-\text{H21A} \cdots \text{O1}$	0.85 (3)	1.86 (3)	2.7093 (18)	177 (2)
$\text{O5}-\text{H5B} \cdots \text{O22}^{\text{iv}}$	0.77 (3)	2.02 (3)	2.784 (2)	172 (2)
$\text{O5}-\text{H5A} \cdots \text{O23}^{\text{v}}$	0.83 (3)	1.88 (3)	2.706 (2)	173 (3)
$\text{O23}-\text{H23B} \cdots \text{O3}^{\text{vi}}$	0.78 (3)	2.06 (3)	2.8302 (19)	172 (3)
$\text{O22}-\text{H22B} \cdots \text{O21}$	0.83 (3)	1.97 (3)	2.794 (2)	177 (3)
$\text{O23}-\text{H23A} \cdots \text{O22}$	0.85 (3)	2.13 (3)	2.959 (2)	165 (2)
$\text{O22}-\text{H22A} \cdots \text{N1}^{\text{vii}}$	0.79 (3)	2.59 (3)	3.152 (2)	130 (2)
$\text{O22}-\text{H22A} \cdots \text{N4}^{\text{vi}}$	0.79 (3)	2.68 (3)	3.242 (2)	130 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Crystal Impact, 2009); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

The Ferdowsi University of Mashhad and Masaryk University are gratefully acknowledged by the authors.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2043).

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Acta Cryst. (2010). E66, m1320-m1321 [doi:10.1107/S1600536810037736]

Bis(2-amino-4-methylpyrimidin-3-ium) *trans*-diaquabis(pyrazine-2,3-dicarboxylato)cobaltate(II) hexahydrate

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Comment

Many organic aromatic ligands and metal ions may aggregate into supramolecular networks using coordination and hydrogen bonds and π – π stacking interactions. Metal pyrazine-(di)carboxylates may possess versatile structural motifs, which finally aggregate to various supramolecular architectures with interesting properties. For the first time, Takusagawa & Shimada (1973) determined the structure of pyzdcH₂. Until now, several proton transfer compounds with pyzdcH₂ have been synthesized by our research group such as, (ampyH)₂[M(pyzdc)₂(H₂O)₂].6H₂O (*M* = Co (**1**), Cu, Zn and ampy = 2-amino-4-methyl pyridine) (Eshtiagh-Hosseini *et al.*, 2010*b,cd*). Continuing our previous work on the syntheses of coordination compounds *via* proton transfer mechanism, we planned the reaction between pyzdcH₂, ampym and cobalt^{II} chloride in order to provide a new coordination compound containing a proton transfer ligand. The title compound, (ampymH)₂[Co(pyzdcH)₂(H₂O)₂].6H₂O, is analogous to previously synthesized compound **1** in which ampy was replaced by ampym (Fig. 1). The equatorial plane is occupied by two (pyzdc)²⁻ ligands coordinating through the pyrazine nitrogen and one oxygen of the deprotonated carboxylate groups. The two coordinated water molecules occupy the axial plane. This compound consists of an anionic moiety, *trans*-[Co(pyzdc)₂(H₂O)₂]²⁻ complex, counter-ions, (ampymH)⁺, and six uncoordinated water molecules. The Co—O and Co—N bond distances related to the (pyzdc)²⁻ ligand are 2.0445 (12) Å, and 2.1086 (14) Å, respectively. The intermolecular forces between the anionic, cationic parts, and uncoordinated water molecules consist of hydrogen bonding interactions. The hydrogen bond interactions cause further stabilization for crystalline network using two types of graph-sets namely *R*²₂(8) and *R*⁴₆(12) (Fig. 2). Indeed, the arrangement of anionic parts in the network resulted in the creation of anionic holes for entering cationic parts; this arrangement results in off-set or slipped π – π stacking interactions with the distance of 3.6337 (9) Å between the centroids of the rings (Fig. 3). Moreover, six uncoordinated water molecules increase the number of hydrogen bonds in the crystalline network and lead to the formation of (H₂O)_{*n*} clusters throughout the crystalline network (Aghabozorg *et al.* 2010).

Experimental

A solution of pyzdcH₂ (0.60 mmol, 0.10 g), ampym (1.2 mmol, 0.13 g), and CoCl₂.6H₂O (0.02 mmol, 0.05 g) at 333 K lead to formation of (ampymH)₂[Co(pyzdc)₂(H₂O)₂].6H₂O orange block crystals after slow evaporation of solvent at room temperature.

Refinement

Carbon and nitrogen bound hydrogen atoms were positioned geometrically and refined as riding using standard *SHELXTL* constraints, with their *U*_{iso} set to either 1.2*U*_{eq} or 1.5*U*_{eq} (methyl) of their parent atoms. The C–H distances were set to

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0.95 and 0.98 Å for aromatic and methyl groups, respectively, the N-H distances used were 0.88 Å. Oxygen bound hydrogen atoms were located in a difference Fourier map and refined isotropically.

Figures

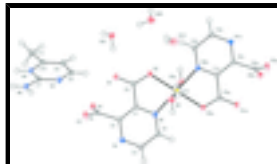


Fig. 1. Molecular structure of (ampymH)₂[Co(pyzdc)₂(H₂O)₂].6H₂O compound. Ellipsoids are drawn at the 50% probability level.

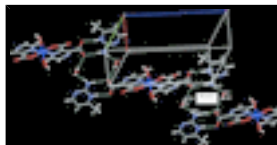


Fig. 2. Schematic representation of the present $R^2_2(8)$ and $R^4_6(12)$ graph-sets in the crystalline network.

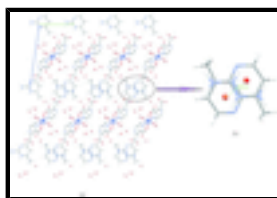


Fig. 3. (a) Packing diagram along the a -axis. (b) The off-set or slipped π - π stacking interactions between aromatic rings of two (ampymH)⁺ fragments.

Bis(2-amino-4-methylpyrimidin-3-ium) *trans*-diaquabis(pyrazine-2,3-dicarboxylato)cobaltate(II) hexahydrate

Crystal data

(C₅H₈N₃)₂[Co(C₆H₂N₂O₄)₂(H₂O)₂].6H₂O

$M_r = 755.54$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 6.5880$ (4) Å

$b = 8.0591$ (5) Å

$c = 15.0285$ (8) Å

$\alpha = 98.085$ (5)°

$\beta = 96.940$ (4)°

$\gamma = 91.261$ (5)°

$V = 783.58$ (8) Å³

$Z = 1$

$F(000) = 393$

$D_x = 1.601$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4417 reflections

$\theta = 3.1$ – 27.6 °

$\mu = 0.64$ mm⁻¹

$T = 120$ K

Plate, pale orange

$0.40 \times 0.40 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur

diffractometer with Sapphire2 (large Be window) detector 2758 independent reflections

Radiation source: Enhance (Mo) X-ray Source graphite

2428 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.011$

Detector resolution: 8.4353 pixels mm⁻¹

$\theta_{\text{max}} = 25.0$ °, $\theta_{\text{min}} = 3.1$ °

ω scan

$h = -7 \rightarrow 7$

Absorption correction: multi-scan

$k = -9 \rightarrow 9$

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.903$, $T_{\max} = 1.000$

$l = -17 \rightarrow 17$

5733 measured reflections

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.025$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.064$

H atoms treated by a mixture of independent and constrained refinement

$S = 1.04$

$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.458P]$

where $P = (F_o^2 + 2F_c^2)/3$

2758 reflections

$(\Delta/\sigma)_{\max} < 0.001$

256 parameters

$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$

0 restraints

$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co2	0.5000	0.5000	0.5000	0.01426 (11)
O1	0.58615 (17)	0.62856 (14)	0.25548 (7)	0.0143 (3)
O2	0.62546 (18)	0.51362 (15)	0.38308 (8)	0.0167 (3)
O3	0.33723 (18)	0.93937 (14)	0.19964 (8)	0.0163 (3)
O4	0.17222 (18)	0.69382 (14)	0.14483 (8)	0.0144 (3)
O5	0.6551 (2)	0.72932 (17)	0.55885 (9)	0.0201 (3)
H5A	0.572 (4)	0.793 (3)	0.5817 (18)	0.053 (8)*
H5B	0.748 (4)	0.733 (3)	0.5952 (17)	0.037 (8)*
N1	0.0477 (2)	0.84612 (18)	0.33031 (9)	0.0150 (3)
N2	0.2829 (2)	0.64620 (17)	0.43486 (9)	0.0136 (3)
N3	0.7241 (2)	0.96452 (17)	-0.03740 (9)	0.0115 (3)
H3A	0.7142	1.0023	-0.0898	0.014*
N4	0.7962 (2)	1.02237 (18)	0.12227 (9)	0.0142 (3)
N5	0.8275 (2)	1.23050 (17)	0.03349 (9)	0.0132 (3)

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H5C	0.8654	1.3024	0.0827	0.016*
H5D	0.8193	1.2640	-0.0201	0.016*
C1	0.3367 (2)	0.6769 (2)	0.35513 (11)	0.0111 (3)
C2	0.2154 (3)	0.7745 (2)	0.30243 (11)	0.0114 (3)
C3	-0.0026 (3)	0.8140 (2)	0.40958 (11)	0.0154 (4)
H3	-0.1212	0.8619	0.4311	0.018*
C4	0.1129 (3)	0.7127 (2)	0.46163 (11)	0.0150 (4)
H4	0.0704	0.6903	0.5171	0.018*
C5	0.5328 (2)	0.6005 (2)	0.32850 (11)	0.0115 (4)
C6	0.2498 (2)	0.8028 (2)	0.20784 (11)	0.0123 (4)
C7	0.7832 (2)	1.0727 (2)	0.03993 (11)	0.0115 (4)
C8	0.7472 (3)	0.8626 (2)	0.12403 (12)	0.0157 (4)
H8	0.7518	0.8251	0.1814	0.019*
C9	0.6893 (3)	0.7459 (2)	0.04676 (12)	0.0158 (4)
H9	0.6572	0.6322	0.0514	0.019*
C10	0.6801 (2)	0.7997 (2)	-0.03562 (12)	0.0133 (4)
C11	0.6237 (3)	0.6941 (2)	-0.12543 (12)	0.0174 (4)
H11A	0.7309	0.7070	-0.1641	0.026*
H11B	0.4936	0.7298	-0.1542	0.026*
H11C	0.6096	0.5762	-0.1170	0.026*
O21	0.9070 (2)	0.46146 (16)	0.19544 (9)	0.0162 (3)
O22	0.9951 (2)	0.2292 (2)	0.31495 (9)	0.0216 (3)
O23	0.6098 (2)	0.07554 (19)	0.35418 (10)	0.0228 (3)
H21A	0.809 (4)	0.516 (3)	0.2147 (16)	0.039 (7)*
H21B	0.987 (4)	0.530 (3)	0.1837 (15)	0.030 (6)*
H22A	1.001 (4)	0.142 (4)	0.2846 (18)	0.054 (9)*
H22B	0.973 (4)	0.300 (3)	0.2803 (18)	0.049 (8)*
H23A	0.708 (4)	0.136 (3)	0.3438 (17)	0.048 (8)*
H23B	0.544 (4)	0.039 (3)	0.3088 (19)	0.049 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co2	0.01444 (19)	0.0194 (2)	0.01064 (18)	0.00400 (14)	0.00278 (13)	0.00658 (13)
O1	0.0159 (6)	0.0177 (6)	0.0109 (6)	0.0020 (5)	0.0042 (5)	0.0054 (5)
O2	0.0164 (6)	0.0223 (7)	0.0138 (6)	0.0075 (5)	0.0041 (5)	0.0085 (5)
O3	0.0210 (7)	0.0146 (6)	0.0137 (6)	-0.0042 (5)	-0.0001 (5)	0.0054 (5)
O4	0.0175 (6)	0.0148 (6)	0.0108 (6)	-0.0018 (5)	0.0004 (5)	0.0026 (5)
O5	0.0173 (7)	0.0245 (8)	0.0181 (7)	0.0034 (6)	0.0006 (6)	0.0024 (6)
N1	0.0146 (7)	0.0163 (8)	0.0137 (7)	0.0023 (6)	0.0008 (6)	0.0018 (6)
N2	0.0142 (7)	0.0164 (8)	0.0105 (7)	0.0000 (6)	0.0017 (6)	0.0027 (6)
N3	0.0122 (7)	0.0132 (7)	0.0100 (7)	0.0011 (6)	0.0021 (6)	0.0040 (6)
N4	0.0136 (7)	0.0171 (8)	0.0127 (7)	0.0004 (6)	0.0016 (6)	0.0054 (6)
N5	0.0172 (8)	0.0141 (8)	0.0083 (7)	-0.0014 (6)	0.0001 (6)	0.0030 (6)
C1	0.0128 (8)	0.0110 (8)	0.0095 (8)	-0.0017 (6)	0.0006 (7)	0.0019 (6)
C2	0.0127 (8)	0.0095 (8)	0.0112 (8)	-0.0025 (6)	0.0005 (7)	0.0003 (6)
C3	0.0141 (9)	0.0179 (9)	0.0139 (9)	0.0023 (7)	0.0028 (7)	0.0002 (7)
C4	0.0153 (9)	0.0193 (9)	0.0109 (8)	0.0003 (7)	0.0042 (7)	0.0018 (7)

C5	0.0128 (8)	0.0101 (8)	0.0113 (9)	-0.0009 (7)	0.0003 (7)	0.0011 (7)
C6	0.0104 (8)	0.0145 (9)	0.0130 (9)	0.0041 (7)	0.0011 (7)	0.0050 (7)
C7	0.0067 (8)	0.0162 (9)	0.0120 (8)	0.0019 (7)	0.0019 (7)	0.0028 (7)
C8	0.0110 (8)	0.0228 (10)	0.0156 (9)	0.0029 (7)	0.0022 (7)	0.0102 (7)
C9	0.0130 (9)	0.0140 (9)	0.0217 (10)	0.0004 (7)	0.0023 (7)	0.0071 (7)
C10	0.0075 (8)	0.0145 (9)	0.0182 (9)	0.0014 (7)	0.0027 (7)	0.0027 (7)
C11	0.0189 (9)	0.0145 (9)	0.0185 (9)	0.0009 (7)	0.0032 (7)	0.0006 (7)
O21	0.0162 (7)	0.0146 (7)	0.0184 (7)	-0.0007 (6)	0.0054 (5)	0.0013 (5)
O22	0.0257 (8)	0.0183 (7)	0.0198 (7)	0.0030 (6)	0.0000 (6)	0.0018 (6)
O23	0.0199 (8)	0.0266 (8)	0.0198 (8)	-0.0015 (6)	0.0007 (6)	-0.0016 (6)

Geometric parameters (Å, °)

Co2—O2 ⁱ	2.0455 (12)	N5—H5C	0.8800
Co2—O2	2.0455 (12)	N5—H5D	0.8800
Co2—N2 ⁱ	2.1101 (14)	C1—C2	1.390 (2)
Co2—N2	2.1101 (14)	C1—C5	1.517 (2)
Co2—O5 ⁱ	2.1167 (14)	C2—C6	1.513 (2)
Co2—O5	2.1167 (14)	C3—C4	1.386 (2)
O1—C5	1.240 (2)	C3—H3	0.9500
O2—C5	1.263 (2)	C4—H4	0.9500
O3—C6	1.259 (2)	C8—C9	1.396 (2)
O4—C6	1.249 (2)	C8—H8	0.9500
O5—H5A	0.83 (3)	C9—C10	1.363 (2)
O5—H5B	0.77 (3)	C9—H9	0.9500
N1—C3	1.332 (2)	C10—C11	1.492 (2)
N1—C2	1.342 (2)	C11—H11A	0.9800
N2—C4	1.334 (2)	C11—H11B	0.9800
N2—C1	1.343 (2)	C11—H11C	0.9800
N3—C10	1.358 (2)	O21—H21A	0.85 (3)
N3—C7	1.361 (2)	O21—H21B	0.81 (2)
N3—H3A	0.8800	O22—H22A	0.79 (3)
N4—C8	1.325 (2)	O22—H22B	0.83 (3)
N4—C7	1.349 (2)	O23—H23A	0.85 (3)
N5—C7	1.318 (2)	O23—H23B	0.78 (3)
O2 ⁱ —Co2—O2	180.0	C1—C2—C6	124.49 (15)
O2 ⁱ —Co2—N2 ⁱ	80.00 (5)	N1—C3—C4	121.94 (16)
O2—Co2—N2 ⁱ	100.00 (5)	N1—C3—H3	119.0
O2 ⁱ —Co2—N2	100.00 (5)	C4—C3—H3	119.0
O2—Co2—N2	80.00 (5)	N2—C4—C3	120.86 (16)
N2 ⁱ —Co2—N2	180.000 (1)	N2—C4—H4	119.6
O2 ⁱ —Co2—O5 ⁱ	89.61 (5)	C3—C4—H4	119.6
O2—Co2—O5 ⁱ	90.39 (5)	O1—C5—O2	126.40 (15)
N2 ⁱ —Co2—O5 ⁱ	86.62 (6)	O1—C5—C1	117.16 (14)
N2—Co2—O5 ⁱ	93.38 (6)	O2—C5—C1	116.44 (14)
O2 ⁱ —Co2—O5	90.39 (5)	O4—C6—O3	126.31 (15)

supplementary materials

O2—Co2—O5	89.61 (5)	O4—C6—C2	116.05 (14)
N2 ⁱ —Co2—O5	93.38 (6)	O3—C6—C2	117.32 (14)
N2—Co2—O5	86.62 (6)	N5—C7—N4	119.64 (15)
O5 ⁱ —Co2—O5	180.00 (7)	N5—C7—N3	118.68 (15)
C5—O2—Co2	116.20 (10)	N4—C7—N3	121.68 (15)
Co2—O5—H5A	108.8 (19)	N4—C8—C9	124.00 (16)
Co2—O5—H5B	121.8 (18)	N4—C8—H8	118.0
H5A—O5—H5B	105 (3)	C9—C8—H8	118.0
C3—N1—C2	116.87 (15)	C10—C9—C8	118.16 (16)
C4—N2—C1	118.22 (14)	C10—C9—H9	120.9
C4—N2—Co2	130.55 (12)	C8—C9—H9	120.9
C1—N2—Co2	111.19 (11)	N3—C10—C9	117.89 (15)
C10—N3—C7	121.63 (14)	N3—C10—C11	116.07 (15)
C10—N3—H3A	119.2	C9—C10—C11	126.04 (16)
C7—N3—H3A	119.2	C10—C11—H11A	109.5
C8—N4—C7	116.59 (15)	C10—C11—H11B	109.5
C7—N5—H5C	120.0	H11A—C11—H11B	109.5
C7—N5—H5D	120.0	C10—C11—H11C	109.5
H5C—N5—H5D	120.0	H11A—C11—H11C	109.5
N2—C1—C2	120.13 (15)	H11B—C11—H11C	109.5
N2—C1—C5	116.11 (14)	H21A—O21—H21B	106 (2)
C2—C1—C5	123.75 (14)	H22A—O22—H22B	107 (3)
N1—C2—C1	121.91 (15)	H23A—O23—H23B	110 (3)
N1—C2—C6	113.51 (14)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3A \cdots O3 ⁱⁱ	0.88	1.77	2.6487 (17)	172
N5—H5C \cdots O21 ⁱⁱⁱ	0.88	1.96	2.8350 (18)	172
N5—H5D \cdots O4 ⁱⁱ	0.88	1.96	2.8310 (18)	171
O21—H21B \cdots O4 ^{iv}	0.81 (2)	1.97 (3)	2.7777 (18)	175 (2)
O21—H21A \cdots O1	0.85 (3)	1.86 (3)	2.7093 (18)	177 (2)
O5—H5B \cdots O22 ^v	0.77 (3)	2.02 (3)	2.784 (2)	172 (2)
O5—H5A \cdots O23 ⁱ	0.83 (3)	1.88 (3)	2.706 (2)	173 (3)
O23—H23B \cdots O3 ^{vi}	0.78 (3)	2.06 (3)	2.8302 (19)	172 (3)
O22—H22B \cdots O21	0.83 (3)	1.97 (3)	2.794 (2)	177 (3)
O23—H23A \cdots O22	0.85 (3)	2.13 (3)	2.959 (2)	165 (2)
O22—H22A \cdots N1 ^{vii}	0.79 (3)	2.59 (3)	3.152 (2)	130 (2)
O22—H22A \cdots N4 ^{vi}	0.79 (3)	2.68 (3)	3.242 (2)	130 (2)

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

Fig. 1

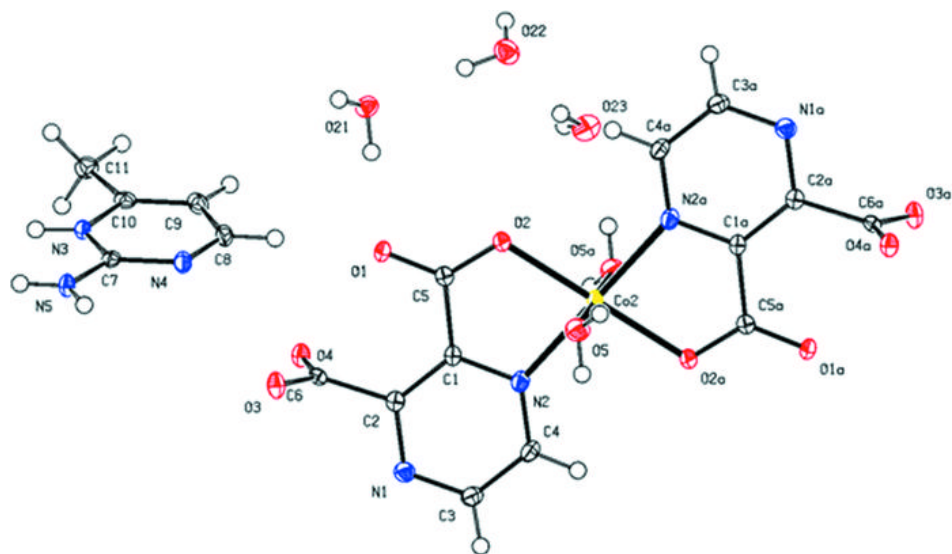


Fig. 3

