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Structure Reports

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trans-Tetraaquabis[3-(3-pyridyl)acrylato- κ N]cobalt(II)Jozef Miklovič,^a Jan Moncol,^{b*} Dušan Mikloš,^b Peter Segľa^b and Marian Koman^b

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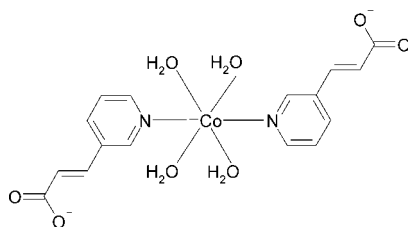
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.156; data-to-parameter ratio = 20.4.

The asymmetric unit of the title compound, $[\text{Co}(\text{C}_8\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_4]$, contains one half-molecule. The Co^{II} atom lies on an inversion centre and is coordinated by two N atoms of the pyridine rings of 3-(3-pyridyl)acrylate anions and four O atoms of water molecules in a distorted octahedral coordination geometry. In the crystal structure, intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules, forming a three-dimensional network.

Related literature

For related literature, see: Ayyappan *et al.* (2001); Kurmoo *et al.* (2005); Tong *et al.* (2003); Zhou *et al.* (2006); For related structures, see: Huang *et al.* (2005); Tang *et al.* (2006); Yang *et al.* (2006).



Experimental

Crystal data

$[\text{Co}(\text{C}_8\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_4]$
 $M_r = 427.27$
Monoclinic, $P2_1/n$
 $a = 11.235$ (1) Å
 $b = 7.020$ (1) Å
 $c = 12.012$ (1) Å
 $\beta = 112.81$ (1)°

$V = 873.29$ (18) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.03$ mm⁻¹
 $T = 294$ (2) K
0.40 × 0.25 × 0.20 mm

Data collection

Siemens P4 diffractometer

Absorption correction: ψ scan
(*XEMP*; Siemens, 1994)
 $T_{\text{min}} = 0.672$, $T_{\text{max}} = 0.808$

3307 measured reflections
2533 independent reflections
2255 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

3 standard reflections
every 97 reflections
intensity decay: 2.5%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.156$
 $S = 1.10$
2533 reflections

124 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.84$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co—O1W	2.0895 (16)	Co—N1	2.1765 (18)
Co—O2W	2.1061 (16)		
O1W—Co—O2W	89.02 (6)	O2W—Co—N1	87.20 (7)
O1W—Co—N1	90.78 (7)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—H3W \cdots O2 ⁱ	0.82	1.95	2.764 (3)	175
O2W—H4W \cdots O2 ⁱⁱ	0.82	1.95	2.741 (2)	161
O1W—H2W \cdots O1 ⁱ	0.82	1.86	2.678 (2)	175
O1W—H1W \cdots O2 ⁱⁱⁱ	0.82	2.00	2.798 (2)	163

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2421).

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supporting information

Acta Cryst. (2008). E64, m426 [doi:10.1107/S1600536808002559]

***trans*-Tetraaquabis[3-(3-pyridyl)acrylato- κ N]cobalt(II)**

Jozef Miklovič, Jan Moncol, Dušan Mikloš, Peter Segl'a and Marian Koman

S1. Comment

Several Co^{II} coordination polymers that contain a bridging 3-(3-pyridyl)-acrylate ligands have been reported recently (Ayyappan *et al.*, 2001; Kurmoo *et al.*, 2005; Tong *et al.*, 2003; Zhou *et al.*, 2006). However, if the 3-(3-pyridyl)-acrylate anions are coordinated only as terminal ligands, the possibility of participating in a hydrogen-bonding network originates. As part of our efforts to investigate metal(II) complexes based on pyridyl- carboxylic acids, we report herein the crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) Co^{II} atom lies on an inversion centre and adopts a distorted octahedral coordination geometry with two N atoms of the pyridine rings of 3-(3-pyridyl)-acrylate anions and four O atoms of water molecules (Table 1), where the two symmetry related 3-(3-pyridyl)-acrylate ligands are in *trans* positions.

The bond lengths and angles may be compared with the corresponding values in [Co(C₈H₆NO₂)₂(H₂O)₄].2H₂O [(II); Huang *et al.*, 2005]. In (II), Co^{II} atom displays a similar distorted octahedral coordination geometry, but the existence of two more water molecules result in the formation of a different hydrogen-bonding network. On the other hand, complex (I) is isostructural with [Zn(C₈H₆NO₂)₂(H₂O)₄] [(III); Tang *et al.*, 2006; Yang *et al.*, 2006] and [Mn(C₈H₆NO₂)₂(H₂O)₄] [(IV); Huang *et al.*, 2005].

In the crystal structure, intermolecular O—H...O hydrogen bonds (Table 2) link the molecules to form a three-dimensional network.

S2. Experimental

Well shaped crystals of (I) suitable for X-ray analysis were prepared in an H-tube. In the first part of the H-tube, there was aqueous solutions of sodium salt of 3-(3-pyridyl)-acrylic acid and in the second part, there was aqueous solution of Co(II) sulfate. The crystals formed after one month, they were separated and dried at room temperature (yield; 75%). The Anal. Calc.: C, 44.98; H, 6.61; N, 6.56; Co, 13.79; Found: C, 44.72; H, 6.31; N, 6.40; Co, 13.45. IR data (KBr) cm⁻¹: 1646m ν (C=C); 1547vs ν_{as} (COO⁻); 1371vs,br ν_s (COO⁻); 649m δ (py); 415m χ (py). Electronic data (cm⁻¹): 20200; 21200s h; 9100br.

S3. Refinement

H atoms were positioned geometrically with O—H = 0.82 Å (for OH₂ and their displacement parameters were kept fixed as $U_{iso} = 0.032 \text{ \AA}^2$) and C—H = 0.93 Å, for aromatic H atoms and constrained to ride on their parent atoms, with $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$.

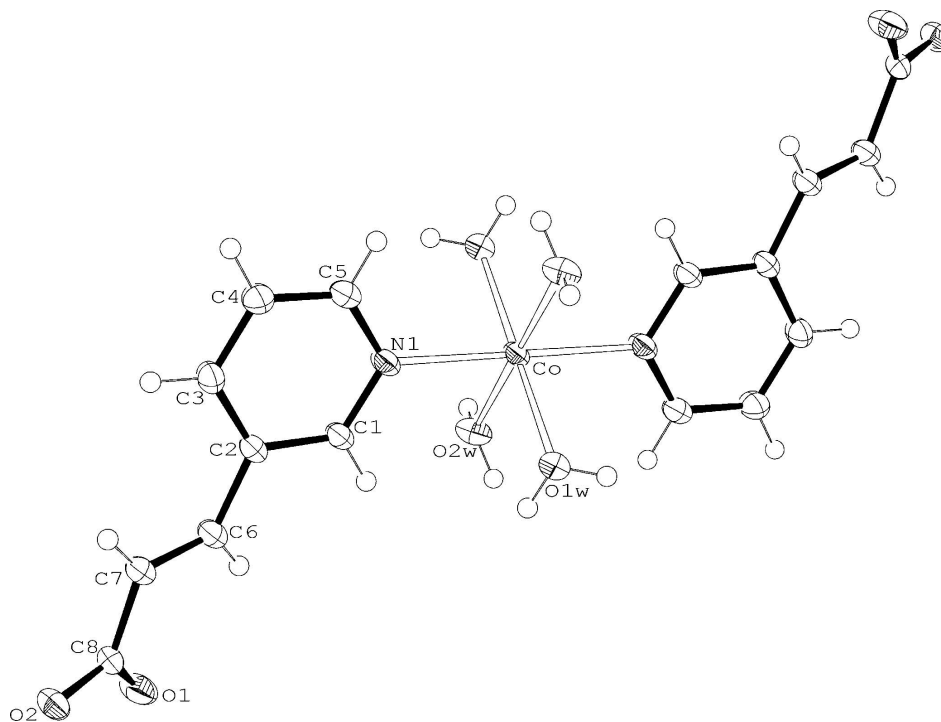


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level

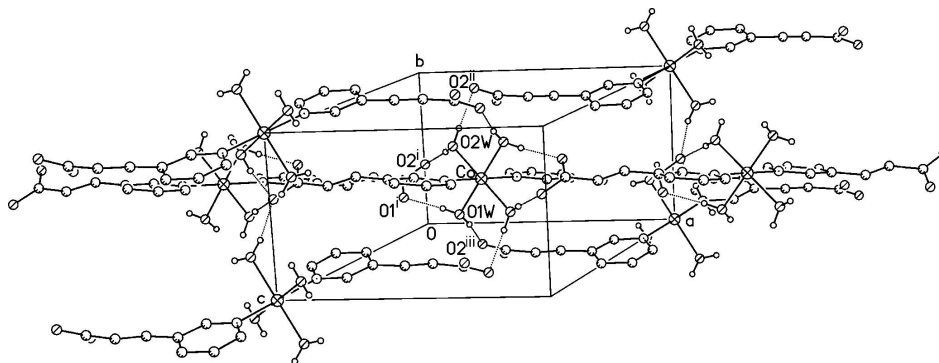


Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines [symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x + 1/2, -y + 3/2, z - 1/2$; (iii) $x + 1/2, -y + 1/2, z - 1/2$].

***trans*-Tetraaquabis[3-(3-pyridyl)acrylate- κ N]cobalt(II)**

Crystal data

[Co(C₈H₆NO₂)₂(H₂O)₄]

$M_r = 427.27$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1 n$

$a = 11.235 (1) \text{ \AA}$

$b = 7.020 (1) \text{ \AA}$

$c = 12.012 (1) \text{ \AA}$

$\beta = 112.81 (1)^\circ$

$V = 873.29 (18) \text{ \AA}^3$

$Z = 2$

$F(000) = 442$

$D_x = 1.625 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 25 reflections

$\theta = 2.5\text{--}8.7^\circ$
 $\mu = 1.03\text{ mm}^{-1}$
 $T = 294\text{ K}$

Block, pink
 $0.40 \times 0.25 \times 0.20\text{ mm}$

Data collection

Siemens P4
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $2\theta/\omega$ scans
 Absorption correction: ψ scan
 (XEMP; Siemens, 1994)
 $T_{\min} = 0.672$, $T_{\max} = 0.808$
 3307 measured reflections

2533 independent reflections
 2255 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 2.1^\circ$
 $h = -1 \rightarrow 15$
 $k = -1 \rightarrow 9$
 $l = -16 \rightarrow 15$
 3 standard reflections every 97 reflections
 intensity decay: 2.5%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.156$
 $S = 1.10$
 2533 reflections
 124 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
 $w = 1/[\sigma^2(F_o^2) + (0.1034P)^2 + 0.5011P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.65\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.84\text{ e \AA}^{-3}$

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	$U_{\text{iso}}^*/U_{\text{eq}}$
Co	0.5000	0.5000	0.5000	0.01873 (16)
N1	0.44388 (17)	0.5543 (3)	0.65137 (17)	0.0228 (4)
O1	-0.13338 (15)	0.6559 (3)	0.61120 (16)	0.0328 (4)
O2	-0.12936 (18)	0.5143 (2)	0.77834 (18)	0.0264 (4)
O1W	0.38329 (15)	0.2573 (2)	0.45303 (14)	0.0257 (3)
H1W	0.3959	0.1739	0.4111	0.032*
H2W	0.3072	0.2884	0.4306	0.032*
O2W	0.33927 (15)	0.6646 (2)	0.39394 (15)	0.0270 (3)
H3W	0.2800	0.6092	0.3407	0.032*
H4W	0.3567	0.7701	0.3751	0.032*
C1	0.3185 (2)	0.5672 (3)	0.63318 (19)	0.0236 (4)
H1	0.2578	0.5545	0.5546	0.028*

C2	0.27363 (19)	0.5986 (3)	0.72477 (19)	0.0217 (4)
C3	0.3653 (2)	0.6228 (3)	0.84170 (19)	0.0248 (4)
H3	0.3400	0.6463	0.9055	0.030*
C4	0.4946 (2)	0.6114 (4)	0.86108 (19)	0.0273 (4)
H4	0.5574	0.6271	0.9384	0.033*
C5	0.5303 (2)	0.5765 (3)	0.7649 (2)	0.0243 (4)
H5	0.6177	0.5681	0.7795	0.029*
C6	0.1337 (2)	0.6061 (3)	0.69088 (19)	0.0238 (4)
H6	0.0838	0.6301	0.6100	0.029*
C7	0.0699 (2)	0.5824 (3)	0.7628 (2)	0.0249 (4)
H7	0.1153	0.5635	0.8452	0.030*
C8	-0.07372 (19)	0.5859 (3)	0.71227 (19)	0.0216 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0127 (2)	0.0260 (2)	0.0190 (2)	-0.00015 (12)	0.00773 (16)	-0.00068 (12)
N1	0.0157 (8)	0.0320 (9)	0.0231 (8)	-0.0009 (7)	0.0103 (6)	-0.0001 (7)
O1	0.0190 (7)	0.0495 (10)	0.0296 (8)	-0.0006 (7)	0.0091 (6)	0.0048 (7)
O2	0.0215 (8)	0.0310 (9)	0.0317 (9)	-0.0023 (6)	0.0158 (7)	-0.0007 (6)
O1W	0.0187 (7)	0.0311 (8)	0.0281 (8)	-0.0023 (6)	0.0098 (6)	-0.0046 (6)
O2W	0.0178 (7)	0.0323 (8)	0.0292 (8)	-0.0012 (6)	0.0072 (6)	0.0063 (6)
C1	0.0155 (8)	0.0353 (11)	0.0219 (9)	-0.0015 (8)	0.0092 (7)	-0.0026 (8)
C2	0.0167 (8)	0.0272 (9)	0.0240 (9)	-0.0002 (7)	0.0108 (7)	-0.0010 (7)
C3	0.0220 (9)	0.0341 (11)	0.0209 (9)	0.0016 (8)	0.0111 (8)	-0.0010 (8)
C4	0.0205 (9)	0.0390 (11)	0.0204 (9)	0.0006 (8)	0.0058 (7)	-0.0017 (8)
C5	0.0166 (9)	0.0301 (11)	0.0265 (10)	-0.0004 (8)	0.0086 (8)	-0.0012 (8)
C6	0.0168 (8)	0.0306 (10)	0.0252 (9)	0.0005 (7)	0.0097 (7)	-0.0011 (8)
C7	0.0169 (9)	0.0337 (11)	0.0256 (9)	-0.0012 (8)	0.0098 (7)	-0.0030 (8)
C8	0.0179 (8)	0.0248 (9)	0.0252 (9)	-0.0014 (7)	0.0117 (7)	-0.0046 (7)

Geometric parameters (Å, °)

Co—O1W ⁱ	2.0895 (16)	C1—C2	1.394 (3)
Co—O1W	2.0895 (16)	C1—H1	0.9300
Co—O2W ⁱ	2.1061 (16)	C2—C3	1.393 (3)
Co—O2W	2.1061 (16)	C2—C6	1.465 (3)
Co—N1 ⁱ	2.1765 (18)	C3—C4	1.382 (3)
Co—N1	2.1765 (18)	C3—H3	0.9300
N1—C5	1.342 (3)	C4—C5	1.384 (3)
N1—C1	1.343 (3)	C4—H4	0.9300
O1—C8	1.238 (3)	C5—H5	0.9300
O2—C8	1.288 (3)	C6—C7	1.329 (3)
O1W—H1W	0.82	C6—H6	0.9300
O1W—H2W	0.82	C7—C8	1.488 (3)
O2W—H3W	0.82	C7—H7	0.9300
O2W—H4W	0.82		

O1W ⁱ —Co—O1W	180.0	N1—C1—C2	124.1 (2)
O1W ⁱ —Co—O2W ⁱ	89.02 (6)	N1—C1—H1	118.0
O1W—Co—O2W ⁱ	90.98 (6)	C2—C1—H1	118.0
O1W ⁱ —Co—O2W	90.98 (6)	C3—C2—C1	117.57 (19)
O1W—Co—O2W	89.02 (6)	C3—C2—C6	124.77 (18)
O2W ⁱ —Co—O2W	180.0	C1—C2—C6	117.65 (19)
O1W ⁱ —Co—N1 ⁱ	90.78 (7)	C4—C3—C2	118.75 (19)
O1W—Co—N1 ⁱ	89.22 (7)	C4—C3—H3	120.6
O2W ⁱ —Co—N1 ⁱ	87.20 (7)	C2—C3—H3	120.6
O2W—Co—N1 ⁱ	92.80 (7)	C3—C4—C5	119.7 (2)
O1W ⁱ —Co—N1	89.22 (7)	C3—C4—H4	120.1
O1W—Co—N1	90.78 (7)	C5—C4—H4	120.1
O2W ⁱ —Co—N1	92.80 (7)	N1—C5—C4	122.64 (19)
O2W—Co—N1	87.20 (7)	N1—C5—H5	118.7
N1 ⁱ —Co—N1	180.0	C4—C5—H5	118.7
C5—N1—C1	117.26 (18)	C7—C6—C2	127.3 (2)
C5—N1—Co	122.64 (14)	C7—C6—H6	116.4
C1—N1—Co	120.10 (14)	C2—C6—H6	116.4
Co—O1W—H1W	120.6	C6—C7—C8	120.3 (2)
Co—O1W—H2W	109.7	C6—C7—H7	119.8
H1W—O1W—H2W	113.2	C8—C7—H7	119.8
Co—O2W—H3W	117.2	O1—C8—O2	123.5 (2)
Co—O2W—H4W	114.9	O1—C8—C7	119.73 (19)
H3W—O2W—H4W	115.0	O2—C8—C7	116.8 (2)
O1W ⁱ —Co—N1—C5	-54.14 (19)	C1—C2—C3—C4	-1.1 (3)
O1W—Co—N1—C5	125.86 (19)	C6—C2—C3—C4	179.7 (2)
O2W ⁱ —Co—N1—C5	34.84 (19)	C2—C3—C4—C5	0.0 (4)
O2W—Co—N1—C5	-145.16 (19)	C1—N1—C5—C4	0.0 (4)
O1W ⁱ —Co—N1—C1	125.68 (19)	Co—N1—C5—C4	179.86 (18)
O1W—Co—N1—C1	-54.32 (19)	C3—C4—C5—N1	0.5 (4)
O2W ⁱ —Co—N1—C1	-145.34 (19)	C3—C2—C6—C7	-20.7 (4)
O2W—Co—N1—C1	34.66 (19)	C1—C2—C6—C7	160.2 (2)
C5—N1—C1—C2	-1.2 (4)	C2—C6—C7—C8	-177.2 (2)
Co—N1—C1—C2	178.93 (18)	C6—C7—C8—O1	-17.7 (3)
N1—C1—C2—C3	1.8 (4)	C6—C7—C8—O2	162.4 (2)
N1—C1—C2—C6	-179.0 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—H3W \cdots O2 ⁱⁱ	0.82	1.95	2.764 (3)	175
O2W—H4W \cdots O2 ⁱⁱⁱ	0.82	1.95	2.741 (2)	161
O1W—H2W \cdots O1 ⁱⁱ	0.82	1.86	2.678 (2)	175
O1W—H1W \cdots O2 ^{iv}	0.82	2.00	2.798 (2)	163

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