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Bis(2-aminobenzonitrile)tetraaqua-cobalt(II) dichloride

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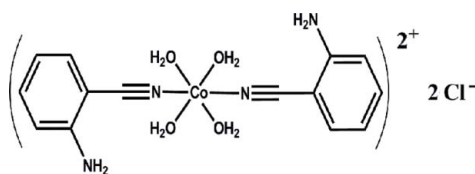
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.034; wR factor = 0.072; data-to-parameter ratio = 19.4.

In the crystal structure of the title compound, $[\text{Co}(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_4]\text{Cl}_2$, the Co^{II} cation lies on an inversion center and is coordinated by two 2-aminobenzonitrile ligands and four water molecules in a distorted octahedral geometry. The Cl^- counter-anion links with the complex cations *via* $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonding. Intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding links the complex cations, forming supramolecular chains running along the b axis.

Related literature

For the chemistry of nitrile derivatives, see: Jin *et al.* (1994); Brewis *et al.* (2003). For a related structure, see: Fu & Zhao (2007).



Experimental

Crystal data

$[\text{Co}(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_4]\text{Cl}_2$
 $M_r = 438.17$

Monoclinic, $P2_1/n$

$a = 12.492$ (3) Å

$b = 6.5864$ (13) Å

$c = 12.608$ (3) Å

$\beta = 109.24$ (3)°

$V = 979.4$ (3) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.17$ mm⁻¹

$T = 298$ K

$0.35 \times 0.30 \times 0.15$ mm

Data collection

Rigaku Mercury2 diffractometer

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

$T_{\text{min}} = 0.732$, $T_{\text{max}} = 0.871$

9255 measured reflections

2227 independent reflections

1872 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.072$

$S = 1.13$

2227 reflections

115 parameters

4 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.30$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O1W	2.0899 (14)	Co1—N1	2.1566 (15)
Co1—O2W	2.0550 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA \cdots Cl1 ⁱ	0.84	2.33	3.1600 (16)	170
O1W—H1WB \cdots Cl1 ⁱⁱ	0.86	2.27	3.1099 (15)	167
O2W—H2WA \cdots N2 ⁱⁱⁱ	0.91	1.99	2.868 (2)	162
O2W—H2WB \cdots Cl1 ^{iv}	0.88	2.27	3.1438 (17)	178
N2—H2B \cdots Cl1 ^v	0.92	2.53	3.4433 (18)	172

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2671).

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supplementary materials

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Bis(2-aminobenzonitrile)tetraaquacobalt(II) dichloride

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Comment

Nitrile derivatives have found wide range of applications in industry and coordination chemistry as ligands. For example, phthalonitriles have been used as starting materials for phthalocyanines (Jin *et al.*, 1994), which are important components for dyes, pigments, gas sensors, optical limiters and liquid crystals, and which are also used in medicine, as singlet oxygen photosensitisers for photodynamic therapy (Brewis *et al.*, 2003). Recently, we have reported a few benzonitrile compounds (Fu & Zhao, 2007). As an extension of our work on the structural characterization, we report here the crystal structure of the title compound tetra-aqua-bis(2-aminobenzonitrile)-cobalt(II) dichloride.

The crystal data show that in the title compound, the Co(II) lies on an inversion center. The distorted octahedral Co(II) environment contains two N atoms from two planar *trans*-related 2-aminobenzonitrile ligands in the axial positions and four aqua O atoms in the equatorial plane. In the crystal, O—H \cdots Cl, N—H \cdots Cl and O—H \cdots N hydrogen bonds generate an infinite two-dimensional network (Fig.1).

Experimental

A mixture of 2-aminobenzonitrile (0.1 mmol) and CoCl₂ (0.1 mmol) and water (1 ml) sealed in a glass tube were maintained at 343 K. Crystals suitable for X-ray analysis were obtained after 5 d.

Refinement

H atoms attached to C atoms were located geometrically and treated as riding with C—H = 0.93 Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms bonded to O and N atoms were located in a difference Fourier map and refined with distance restraints of O—H = 0.85±0.03 and N—H = 0.89±0.03 Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O,N})$.

Figures

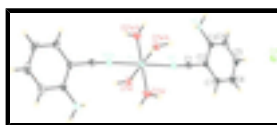


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

Bis(2-aminobenzonitrile)tetraaquacobalt(II) dichloride

Crystal data

[Co(C₇H₆N₂)₂(H₂O)₄]Cl₂

$M_r = 438.17$

Monoclinic, $P2_1/n$

$F(000) = 450$

$D_x = 1.486 \text{ Mg m}^{-3}$

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

supplementary materials

Hall symbol: -P 2yn

$a = 12.492 (3) \text{ \AA}$

$b = 6.5864 (13) \text{ \AA}$

$c = 12.608 (3) \text{ \AA}$

$\beta = 109.24 (3)^\circ$

$V = 979.4 (3) \text{ \AA}^3$

$Z = 2$

Cell parameters from 1872 reflections

$\theta = 3.4\text{--}27.5^\circ$

$\mu = 1.17 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, red

$0.35 \times 0.30 \times 0.15 \text{ mm}$

Data collection

Rigaku Mercury2
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: $13.6612 \text{ pixels mm}^{-1}$

ω scan

Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.732$, $T_{\max} = 0.871$

9255 measured reflections

2227 independent reflections

1872 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.4^\circ$

$h = -16 \rightarrow 16$

$k = -8 \rightarrow 8$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.072$

$S = 1.13$

2227 reflections

115 parameters

4 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

$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 0.2674P]$

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

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

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

$\Delta\rho_{\min} = -0.35 \text{ e \AA}^{-3}$

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	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.5000	0.02435 (11)
Cl1	0.62659 (4)	0.99536 (7)	0.26701 (4)	0.04265 (15)
O1W	-0.10877 (11)	0.0642 (2)	0.33800 (10)	0.0348 (3)
H1WA	-0.1770	0.0308	0.3213	0.052*
H1WB	-0.1014	0.1829	0.3137	0.052*
N2	0.26587 (14)	0.6024 (3)	0.55539 (14)	0.0406 (4)
H2A	0.2560	0.4991	0.5944	0.061*
H2B	0.2997	0.7116	0.5990	0.061*
O2W	0.03539 (12)	-0.2770 (2)	0.44423 (12)	0.0469 (4)
H2WA	0.1036	-0.3409	0.4710	0.070*
H2WB	-0.0087	-0.3427	0.3854	0.070*
C7	0.33808 (16)	0.3068 (3)	0.33515 (15)	0.0366 (4)
H7	0.3225	0.1808	0.3001	0.044*
C2	0.28925 (14)	0.3621 (3)	0.41754 (14)	0.0281 (4)
C3	0.31432 (14)	0.5491 (3)	0.47396 (15)	0.0292 (4)
N1	0.14159 (13)	0.1374 (2)	0.46523 (13)	0.0365 (4)
C5	0.43102 (16)	0.6305 (4)	0.35985 (18)	0.0451 (5)
H5	0.4774	0.7220	0.3393	0.054*
C4	0.38513 (16)	0.6849 (3)	0.44191 (17)	0.0389 (5)
H4	0.4012	0.8116	0.4760	0.047*
C1	0.20887 (15)	0.2307 (3)	0.44319 (15)	0.0297 (4)
C6	0.40921 (17)	0.4417 (4)	0.30739 (17)	0.0436 (5)
H6	0.4424	0.4067	0.2539	0.052*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02442 (18)	0.02295 (18)	0.02613 (18)	-0.00363 (13)	0.00896 (14)	-0.00016 (13)
Cl1	0.0385 (3)	0.0368 (3)	0.0443 (3)	-0.0048 (2)	0.0024 (2)	-0.0060 (2)
O1W	0.0330 (7)	0.0356 (7)	0.0326 (7)	-0.0032 (6)	0.0067 (6)	0.0048 (6)
N2	0.0416 (9)	0.0438 (10)	0.0384 (9)	-0.0046 (8)	0.0157 (8)	-0.0119 (8)
O2W	0.0411 (8)	0.0367 (8)	0.0517 (9)	0.0072 (6)	0.0001 (7)	-0.0150 (7)
C7	0.0305 (10)	0.0490 (12)	0.0309 (10)	0.0002 (9)	0.0110 (8)	-0.0040 (9)
C2	0.0214 (8)	0.0363 (10)	0.0270 (9)	-0.0044 (8)	0.0084 (7)	0.0020 (8)
C3	0.0222 (9)	0.0344 (10)	0.0284 (9)	0.0000 (7)	0.0049 (7)	0.0017 (7)
N1	0.0336 (8)	0.0413 (9)	0.0365 (9)	-0.0094 (8)	0.0139 (7)	0.0002 (7)
C5	0.0287 (10)	0.0601 (14)	0.0461 (12)	-0.0085 (10)	0.0117 (9)	0.0209 (11)
C4	0.0295 (10)	0.0354 (10)	0.0467 (12)	-0.0068 (8)	0.0058 (9)	0.0047 (9)
C1	0.0286 (9)	0.0333 (10)	0.0270 (9)	-0.0031 (8)	0.0089 (8)	-0.0022 (7)
C6	0.0325 (10)	0.0703 (15)	0.0325 (11)	0.0001 (10)	0.0167 (9)	0.0073 (10)

Geometric parameters (\AA , $^\circ$)

Co1—O1W	2.0899 (14)	C7—C6	1.381 (3)
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supplementary materials

Co1—O1W ⁱ	2.0899 (14)	C7—C2	1.415 (2)
Co1—O2W	2.0550 (13)	C7—H7	0.9300
Co1—O2W ⁱ	2.0550 (13)	C2—C3	1.405 (3)
Co1—N1	2.1566 (15)	C2—C1	1.441 (2)
Co1—N1 ⁱ	2.1566 (15)	C3—C4	1.408 (3)
O1W—H1WA	0.8377	N1—C1	1.147 (2)
O1W—H1WB	0.8551	C5—C4	1.385 (3)
N2—C3	1.398 (2)	C5—C6	1.392 (3)
N2—H2A	0.8715	C5—H5	0.9300
N2—H2B	0.9196	C4—H4	0.9300
O2W—H2WA	0.9097	C6—H6	0.9300
O2W—H2WB	0.8784		
O2W—Co1—O2W ⁱ	180.00 (8)	Co1—O2W—H2WB	125.5
O2W—Co1—O1W	89.38 (5)	H2WA—O2W—H2WB	109.6
O2W ⁱ —Co1—O1W	90.62 (5)	C6—C7—C2	119.31 (19)
O2W—Co1—O1W ⁱ	90.62 (5)	C6—C7—H7	120.3
O2W ⁱ —Co1—O1W ⁱ	89.38 (5)	C2—C7—H7	120.3
O1W—Co1—O1W ⁱ	180.00 (5)	C3—C2—C7	121.28 (16)
O2W—Co1—N1	91.13 (6)	C3—C2—C1	117.92 (15)
O2W ⁱ —Co1—N1	88.87 (6)	C7—C2—C1	120.75 (17)
O1W—Co1—N1	91.66 (6)	N2—C3—C2	120.91 (16)
O1W ⁱ —Co1—N1	88.34 (6)	N2—C3—C4	121.11 (17)
O2W—Co1—N1 ⁱ	88.87 (6)	C2—C3—C4	117.90 (17)
O2W ⁱ —Co1—N1 ⁱ	91.13 (6)	C1—N1—Co1	171.82 (16)
O1W—Co1—N1 ⁱ	88.34 (6)	C4—C5—C6	121.43 (18)
O1W ⁱ —Co1—N1 ⁱ	91.66 (6)	C4—C5—H5	119.3
N1—Co1—N1 ⁱ	180.0	C6—C5—H5	119.3
Co1—O1W—H1WA	118.2	C5—C4—C3	120.27 (19)
Co1—O1W—H1WB	115.0	C5—C4—H4	119.9
H1WA—O1W—H1WB	111.8	C3—C4—H4	119.9
C3—N2—H2A	113.3	N1—C1—C2	175.48 (19)
C3—N2—H2B	114.3	C7—C6—C5	119.73 (18)
H2A—N2—H2B	113.3	C7—C6—H6	120.1
Co1—O2W—H2WA	124.4	C5—C6—H6	120.1

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA \cdots C11 ⁱⁱ	0.84	2.33	3.1600 (16)	170.
O1W—H1WB \cdots C11 ⁱⁱⁱ	0.86	2.27	3.1099 (15)	167.
O2W—H2WA \cdots N2 ^{iv}	0.91	1.99	2.868 (2)	162.
O2W—H2WB \cdots C11 ^v	0.88	2.27	3.1438 (17)	178.
N2—H2B \cdots C11 ^{vi}	0.92	2.53	3.4433 (18)	172.

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

