

Intra- and supramolecular interactions in *cis,mer*-diaquatris(1*H*-imidazole- κ N³)-(terephthalato- κ O)cobalt(II) monohydrate

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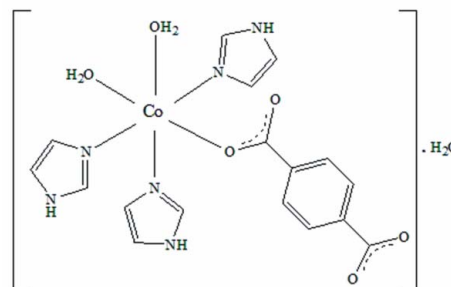
Received 28 February 2012; accepted 20 March 2012

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.029; wR factor = 0.071; data-to-parameter ratio = 15.1.

In the title compound, $[\text{Co}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_3\text{H}_4\text{N}_2)_3(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$, the *cisoid* angles are in the range 85.59 (5)–93.56 (5)°, while two equal *transoid* angles deviate significantly from the ideal linear angle, the third being almost linear. One carboxylate group is almost coplanar [1.23 (13)°] with the plane of its parent aromatic ring, although it has one O-atom donor involved in one coordination and one hydrogen bond as acceptor. The other carboxylate group does not coordinate and is rotated out of this plane with a torsional twist of 17.27 (20)°. The coordination neutral entity, based on aqua ligands and two cyclic co-ligands seems, at first sight, monomeric. Strongly tight, *via* one intramolecular hydrogen bond between aqua and carboxylate O atoms, it brings out a quasi-planar six-membered ring around the Co^{II} atom, turning the CoN₃O₃ coordination octahedron into a new building block. The rigidity of this feature associated with several hydrogen-bonded arrays yields an extended structure. In the resulting supramolecular packing, a binuclear hydrated Co^{II} assembly, built up from triple strands driven by different heterosynthons, embodies the synergy of coordination, covalent and hydrogen bonds.

Related literature

For general background to important structural features inducing some interesting properties, see: Chen *et al.* (1996); Yang *et al.* (2002); Ye & Chen (2003); Xie *et al.* (2009); Baca *et al.* (2003). For related compounds or structures, see: Niu *et al.* (2004); Tong *et al.* (2002); Liu *et al.* (2001, 2003); Zeng *et al.* (1997).



Experimental

Crystal data

$[\text{Co}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_3\text{H}_4\text{N}_2)_3(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$
 $M_r = 481.34$
 Monoclinic, $P2_1/n$
 $a = 7.65363$ (8) Å
 $b = 10.45169$ (13) Å
 $c = 24.7538$ (3) Å

$\beta = 90.227$ (1)°
 $V = 1980.12$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.92$ mm⁻¹
 $T = 291$ K
 $0.21 \times 0.14 \times 0.08$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer
 Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2009)], using a multi-faceted crystal model based on expressions derived by

Clark & Reid (1995)
 $T_{\min} = 0.871$, $T_{\max} = 0.935$
 86135 measured reflections
 4760 independent reflections
 4153 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.071$
 $S = 1.08$
 4760 reflections
 316 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co—O2W	2.1064 (11)	Co—N1	2.1347 (13)
Co—N3	2.1076 (13)	Co—O1	2.1442 (10)
Co—N5	2.1124 (13)	Co—O1W	2.1680 (11)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2N...O1 ⁱ	0.86 (2)	2.09 (2)	2.9204 (17)	162 (2)
N4—H4N...O3W ⁱⁱ	0.85 (2)	2.18 (2)	2.9842 (18)	157.0 (19)
N4—H4N...O4 ⁱⁱⁱ	0.85 (2)	2.50 (2)	2.9521 (18)	114.5 (17)
N6—H6N...O3 ^{iv}	0.84 (2)	2.02 (2)	2.8249 (18)	162 (2)
O1W—H1W...O2	0.85 (3)	1.79 (3)	2.6160 (16)	163 (3)
O1W—H2W...O4 ^v	0.85 (3)	1.85 (3)	2.6606 (16)	161 (2)
O2W—H3W...O3 ^{vi}	0.82 (3)	1.95 (3)	2.7516 (16)	168 (2)
O2W—H4W...O3W ^{vii}	0.82 (2)	2.00 (2)	2.8118 (17)	172 (2)
O3W—H5W...O1W	0.81 (2)	2.08 (2)	2.8632 (16)	164 (2)
O3W—H6W...O3 ^{vi}	0.82 (3)	1.95 (3)	2.7528 (17)	167 (2)

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

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2181).

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supporting information

Acta Cryst. (2012). E68, m480–m481 [https://doi.org/10.1107/S1600536812011993]

Intra- and supramolecular interactions in *cis,mer*-diaquabis(1*H*-imidazole- κ N³) (terephthalato- κ O)cobalt(II) monohydrate

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S1. Comment

This Cobalt-based compound, is the first isomer evidenced, with two aqua ligands *cis* and three N-coordinated imidazole ligands meridional, relative to the Co^{II} centre (Fig.1). Although it is built up from monomeric entity, it exhibits a packing with a relatively interesting metal-metal separation. As shown in Table 1, the Co–Ocarboxylate and the average Co—Ow distances are very closed and are comparable to those observed in related compounds (Niu *et al.*, 2004; Tong *et al.*, 2002). The three independent imidazole groups, and the single terephthalate dianion, both unidentate, participate respectively as donor and acceptor, in strong to moderate hydrogen bonds, and allow the recognition of supramolecular dimensionality (Table 2). The backbone of the architecture is the helical hydrogen-bonded ladder running along *b* axis, composed of alternating $R^4_4(10)$ and $R^3_3(8)$ heterosynthons (Fig.2), which are developed in turn, in bicyclic sheets, both of them containing a six-membered ring, and connected to imidazole ligands *via* secondary N atom. The former is associated with a crossed $R^2_2(6)$ and involves one bifurcated intermolecular H-bond. The latter shares a common Co—O(aqua) bond with a cycle formed of two coordination and three covalent bondings, beside one intramolecular H-bond (Table 2). The resulting quasi-planar six-membered ring, is responsible of environment's rigidity around the metal centre and changes the coordination octahedron in a new building block. The three imidazoles participate as donor with oxygen atom of adjacent carboxylates, and they bring about polymeric chain which mimics the carboxylate-histidine-zinc triad systems (Chen *et al.*, 1996; Yang *et al.*, 2002; Ye *et al.*, 2003; Xie *et al.*, 2009). As seen in Fig.2 and Fig.3, all these overlapping subnetworks lead to the formation of cross-linked supramolecular layers where additional single H-bonds provided by secondary N atom of the imidazoles in one hand, and the spacer of the dicarboxylate on other hand, achieve a well organized three-dimensional packing. Within this three-dimensional framework, the binuclear Co^{II} assembly showing the shortest and probably interesting (Baca *et al.*, 2003) separation metal-metal of 7.6536 (1) Å is built up from triple strand driven by $R^3_3(14)$, $R^4_4(16)$ and $R^5_5(18)$ heterosynthons (Fig.4). A comparison with the two chemically similar Co^{II} compounds [Co(C₃H₄N₂)₄(H₂O)₂](C₈H₄O₄), and [Co(C₃H₄N₂)](C₈H₄O₄).4H₂O (Tong *et al.*, 2002), as well as their isostructural compounds obtained with Mn(II) (Liu *et al.*, 2001;2003) and Cu(II) (Zeng *et al.*, 1997), reveals that their building blocks are mononuclear, and the terephthalate dianion doesn't get involved in coordination. With this study, we may confirm that in this structure, a competition takes place between terephthalate and water and it is probably the presence of both coordinated and uncoordinated water molecules, which builds a new building block, by enhancing the dicarboxylate ligand ability to get involved in coordination sphere.

S2. Experimental

A mixture of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.24 g, 1 mmol), terephthalic acid (0.17 g, 1 mmol), imidazole (0.14 g, 2 mmol) NaOH (0.08 g, 2 mmol) and water (15 ml) was stirred for 30 min at room temperature, then transferred in a 25 ml Teflon-lined stainless steel reactor, then sealed and heated at 120°C for 72 h. Upon cooling to room temperature, light-pink crystals of title compound suitable for X-ray crystallographic analysis were obtained.

S3. Refinement

H atoms attached to C atoms were positioned at calculated positions and were treated as riding on the parent atoms, with $\text{C}-\text{H}=0.95 \text{ \AA}$ and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$. Water hydrogen atoms and H atoms bonded to N atoms were located in a difference map and refined isotropically.

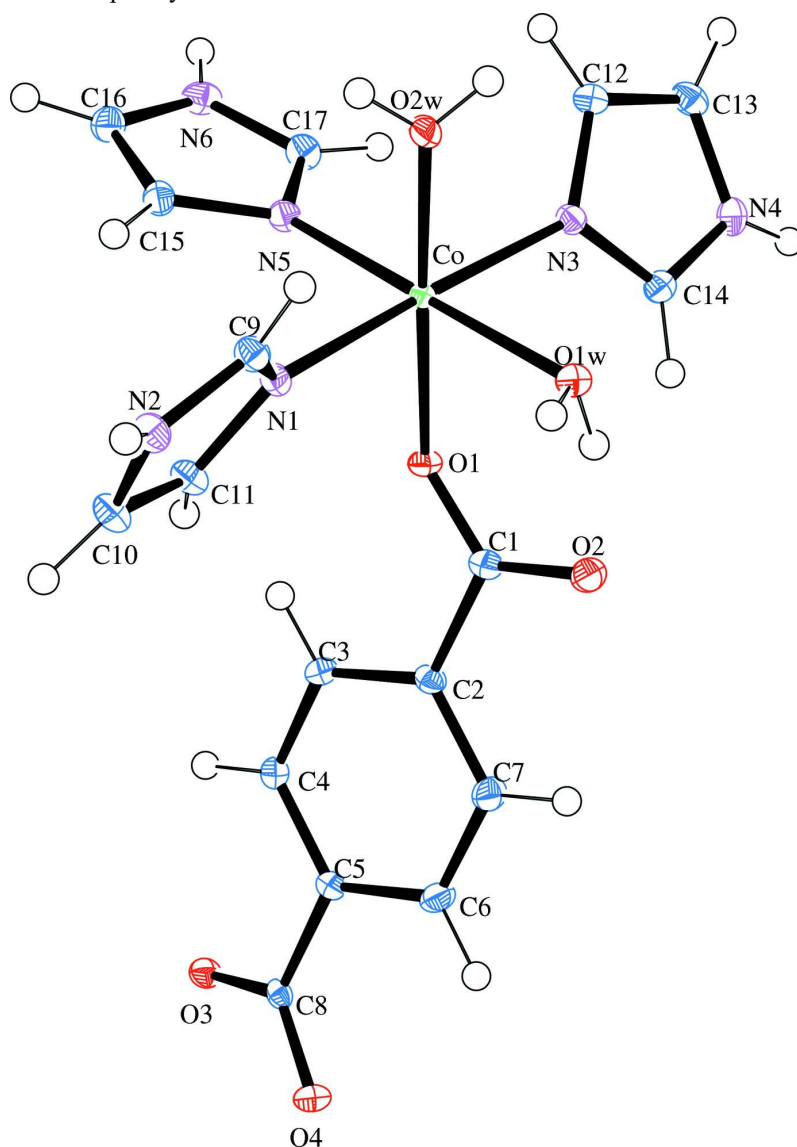


Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

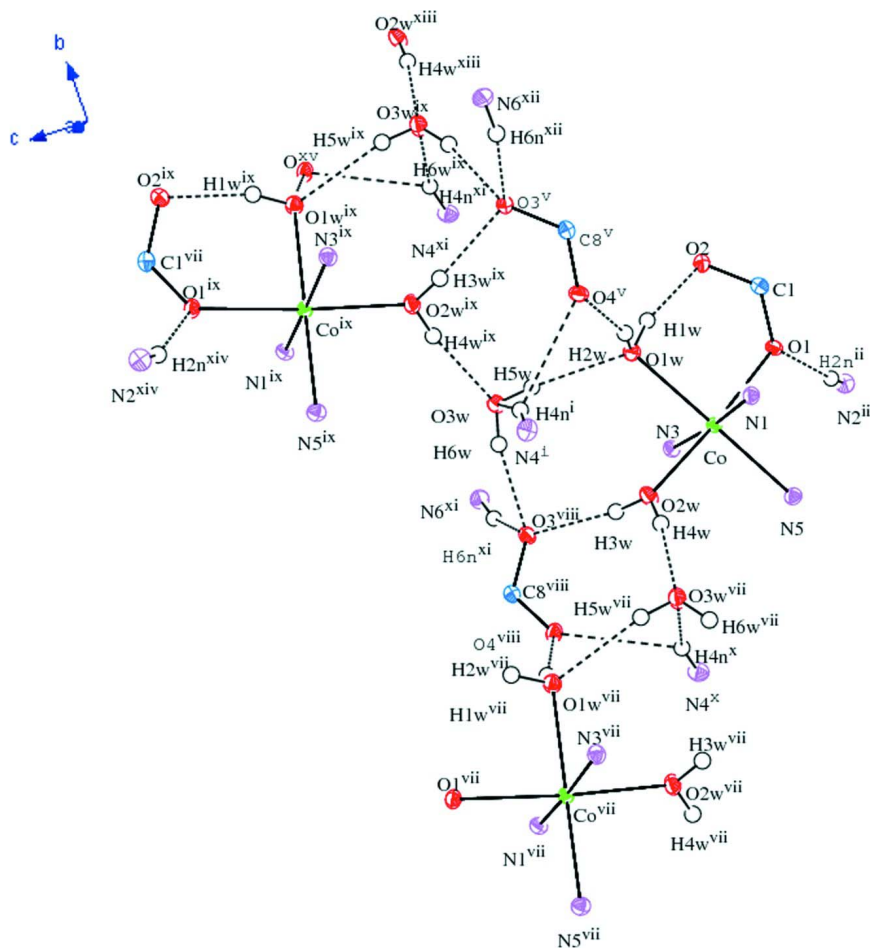


Figure 2

Helical hydrogen-bonded ladder composed of $R^3_3(8)$ and $R^4_4(10)$. Symmetry codes: i: $x + 1, y, z$; ii: $x - 1, y, z$; v: $-x + 1, -y + 1, -z + 1$; vii: $-x + 3/2, y - 1/2, -z + 3/2$; viii: $x - 1/2, -y - 1/2, -z - 1/2$; ix: $-x + 3/2, y + 1/2, -z + 3/2$; x: $-x + 1/2, y - 1/2, -z + 3/2$; xi: $-x + 1/2, y + 1/2, -z + 3/2$; xii: $x + 1, y + 1, z$; xiii: $x, y + 1, z$; xiv: $-x + 5/2, y + 1/2, -z + 3/2$; xv: $x - 1/2, -y + 1/2, z - 1/2$

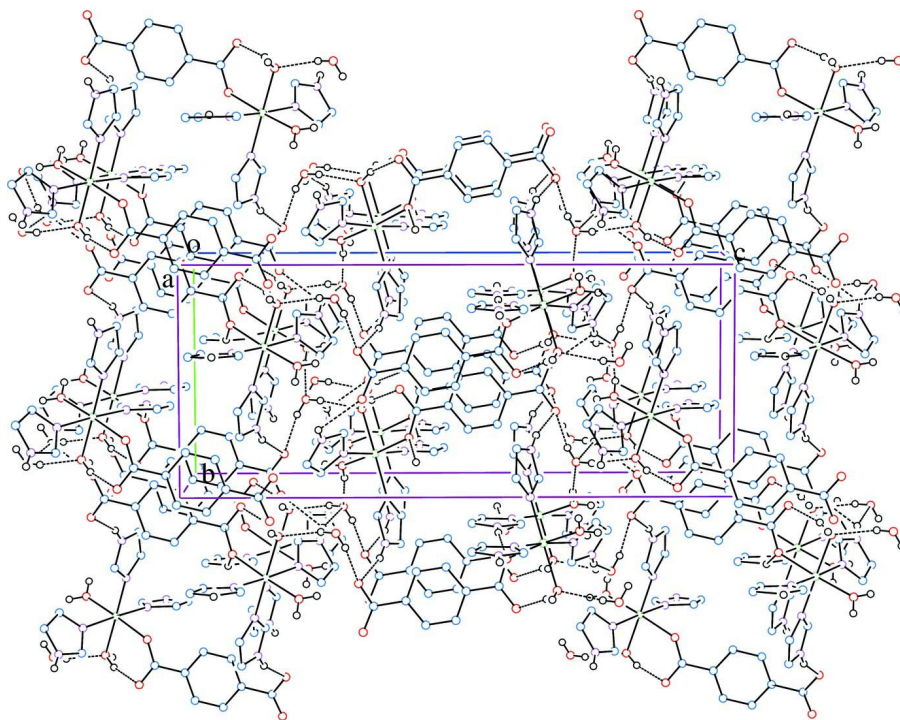


Figure 3

Packing diagram viewed along [100] showing hydrogen bonds and ladder's layers.

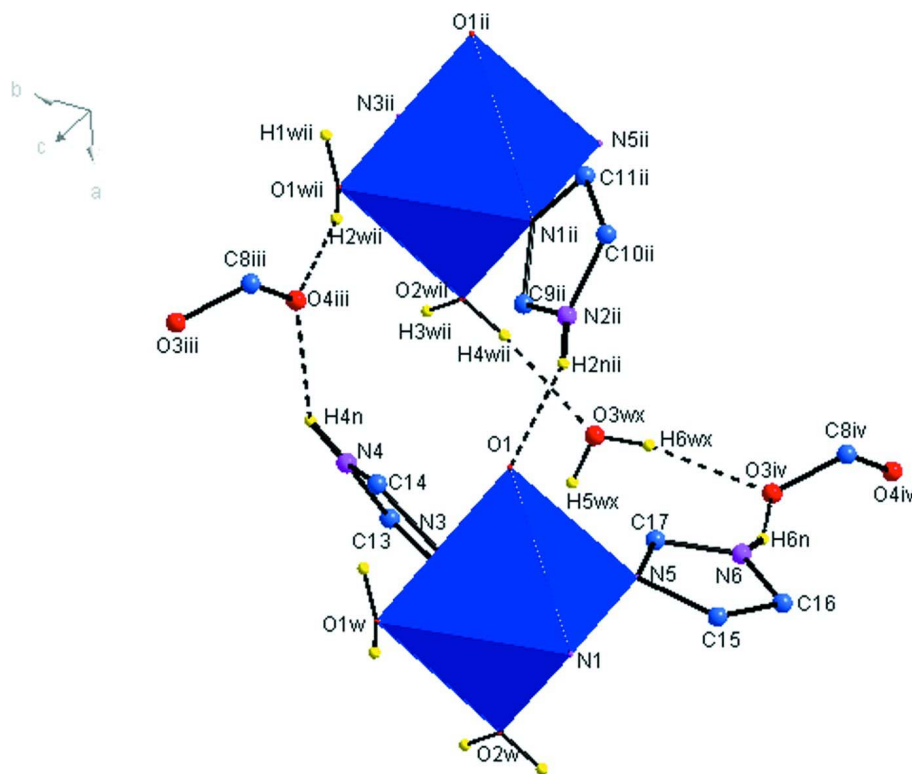


Figure 4

Binuclear Co^{II} assembly with triple strand. Symmetry codes: ii: $x - 1, y, z$; iii: $-x, -y + 1, -z + 1$; iv: $-x, -y, -z + 1$; x: $-x + 1/2, y - 1/2, -z + 3/2$

cis,mer-diaquatrakis(1*H*-imidazole- κ N³)(terephthalato- κ O)cobalt(II) monohydrate

Crystal data

[Co(C₈H₄O₄)(C₃H₄N₂)₃(H₂O)₂] \cdot H₂O

$M_r = 481.34$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 7.65363$ (8) Å

$b = 10.45169$ (13) Å

$c = 24.7538$ (3) Å

$\beta = 90.227$ (1)°

$V = 1980.12$ (4) Å³

$Z = 4$

$F(000) = 996$

$D_x = 1.615$ Mg m⁻³

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

Cell parameters from 35056 reflections

$\theta = 3.3\text{--}32.9^\circ$

$\mu = 0.92$ mm⁻¹

$T = 291$ K

Prism, pink

$0.21 \times 0.14 \times 0.08$ mm

Data collection

Oxford Diffraction Xcalibur
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.4508 pixels mm⁻¹

w σ cans

Absorption correction: analytical

[*CrysAlis RED* (Oxford Diffraction, 2009),

using a multi-faceted crystal model based on

expressions derived by Clark & Reid (1995)]

$T_{\min} = 0.871$, $T_{\max} = 0.935$

86135 measured reflections

4760 independent reflections

4153 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

$\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 3.4^\circ$

$h = -10 \rightarrow 10$

$k = -13 \rightarrow 13$

$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.071$
 $S = 1.08$
 4760 reflections
 316 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 1.5429P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. Absorption correction: CrysAlis RED, Oxford Diffraction (2009) Analytical numerical absorption correction using a multifaceted crystal model based on expressions derived by Clark & Reid (1995).

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. CrysAlis RED, Oxford Diffraction Ltd 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co	0.44254 (2)	0.144772 (19)	0.652633 (8)	0.00874 (6)
O1W	0.52240 (15)	0.33528 (11)	0.67705 (4)	0.0123 (2)
O2W	0.60355 (16)	0.07515 (12)	0.71527 (5)	0.0147 (2)
O3W	0.66608 (15)	0.36561 (12)	0.78325 (5)	0.0149 (2)
O1	0.29257 (14)	0.22971 (10)	0.58868 (4)	0.0115 (2)
O2	0.31457 (15)	0.43979 (11)	0.60544 (4)	0.0165 (2)
O3	0.05014 (14)	0.36582 (10)	0.32226 (4)	0.0130 (2)
O4	0.16128 (14)	0.56111 (11)	0.33113 (4)	0.0134 (2)
C1	0.28701 (19)	0.34725 (15)	0.57476 (6)	0.0116 (3)
C2	0.24336 (19)	0.37422 (15)	0.51627 (6)	0.0115 (3)
C3	0.21121 (19)	0.27458 (15)	0.48037 (6)	0.0115 (3)
H3	0.2188	0.1885	0.4925	0.014*
C4	0.16812 (19)	0.30000 (15)	0.42695 (6)	0.0117 (3)
H4	0.1412	0.2315	0.4031	0.014*
C5	0.16416 (19)	0.42578 (15)	0.40819 (6)	0.0106 (3)
C6	0.2013 (2)	0.52539 (15)	0.44372 (6)	0.0154 (3)
H6	0.2019	0.6111	0.4310	0.018*
C7	0.2375 (2)	0.49999 (16)	0.49776 (6)	0.0160 (3)
H7	0.2584	0.5686	0.5221	0.019*
C8	0.12281 (19)	0.45417 (14)	0.34977 (6)	0.0101 (3)
N1	0.66337 (16)	0.13362 (12)	0.60043 (5)	0.0113 (3)

N2	0.93656 (18)	0.13617 (13)	0.57266 (6)	0.0143 (3)
C9	0.8290 (2)	0.13727 (15)	0.61550 (6)	0.0128 (3)
H9	0.8674	0.1403	0.6520	0.015*
C10	0.8336 (2)	0.13227 (16)	0.52700 (6)	0.0155 (3)
H10	0.8722	0.1310	0.4906	0.019*
C11	0.6653 (2)	0.13062 (15)	0.54460 (6)	0.0143 (3)
H11	0.5647	0.1278	0.5220	0.017*
N3	0.23535 (16)	0.16873 (12)	0.70755 (5)	0.0115 (3)
N4	-0.00080 (18)	0.25190 (14)	0.74341 (5)	0.0145 (3)
C12	0.1779 (2)	0.09015 (16)	0.74877 (6)	0.0146 (3)
H12	0.2327	0.0129	0.7599	0.017*
C13	0.0312 (2)	0.14045 (16)	0.77079 (6)	0.0152 (3)
H13	-0.0359	0.1054	0.7994	0.018*
C14	0.12406 (19)	0.26542 (15)	0.70594 (6)	0.0127 (3)
H14	0.1315	0.3352	0.6815	0.015*
N5	0.36196 (16)	-0.04089 (12)	0.62981 (5)	0.0120 (3)
N6	0.23014 (18)	-0.22776 (14)	0.63208 (6)	0.0157 (3)
C15	0.4649 (2)	-0.13139 (15)	0.60470 (6)	0.0141 (3)
H15	0.5754	-0.1150	0.5888	0.017*
C16	0.3850 (2)	-0.24738 (16)	0.60607 (6)	0.0159 (3)
H16	0.4278	-0.3258	0.5919	0.019*
C17	0.2212 (2)	-0.10428 (16)	0.64582 (6)	0.0147 (3)
H17	0.1262	-0.0667	0.6647	0.018*
H2N	1.048 (3)	0.147 (2)	0.5743 (9)	0.030 (6)*
H4N	-0.088 (3)	0.301 (2)	0.7480 (8)	0.022 (5)*
H6N	0.156 (3)	-0.283 (2)	0.6416 (9)	0.026 (6)*
H1W	0.454 (3)	0.381 (3)	0.6584 (10)	0.043 (7)*
H2W	0.623 (3)	0.360 (2)	0.6673 (9)	0.034 (6)*
H3W	0.576 (3)	0.085 (2)	0.7469 (10)	0.036 (7)*
H4W	0.670 (3)	0.014 (2)	0.7123 (9)	0.029 (6)*
H5W	0.610 (3)	0.365 (2)	0.7556 (9)	0.025 (6)*
H6W	0.639 (3)	0.301 (2)	0.7995 (9)	0.031 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.00883 (10)	0.00915 (11)	0.00823 (10)	-0.00041 (7)	0.00022 (7)	0.00042 (7)
O1W	0.0120 (5)	0.0125 (6)	0.0125 (5)	-0.0014 (4)	-0.0014 (4)	0.0007 (4)
O2W	0.0183 (6)	0.0166 (6)	0.0093 (5)	0.0060 (5)	-0.0001 (4)	0.0001 (4)
O3W	0.0167 (6)	0.0158 (6)	0.0120 (5)	-0.0031 (5)	-0.0020 (5)	0.0025 (5)
O1	0.0127 (5)	0.0111 (5)	0.0107 (5)	-0.0006 (4)	-0.0015 (4)	0.0024 (4)
O2	0.0244 (6)	0.0126 (5)	0.0125 (5)	-0.0002 (5)	-0.0050 (5)	-0.0009 (4)
O3	0.0158 (5)	0.0130 (5)	0.0101 (5)	-0.0024 (4)	-0.0015 (4)	-0.0003 (4)
O4	0.0146 (5)	0.0124 (5)	0.0134 (5)	-0.0022 (4)	-0.0017 (4)	0.0038 (4)
C1	0.0094 (6)	0.0142 (7)	0.0113 (7)	-0.0001 (6)	0.0001 (5)	0.0019 (6)
C2	0.0114 (7)	0.0137 (7)	0.0093 (7)	0.0006 (6)	-0.0007 (5)	0.0011 (6)
C3	0.0116 (7)	0.0103 (7)	0.0127 (7)	0.0001 (5)	-0.0008 (6)	0.0022 (6)
C4	0.0113 (7)	0.0116 (7)	0.0121 (7)	0.0003 (6)	0.0005 (5)	-0.0013 (6)

C5	0.0095 (6)	0.0125 (7)	0.0098 (7)	-0.0001 (5)	0.0000 (5)	0.0006 (6)
C6	0.0218 (8)	0.0101 (7)	0.0141 (7)	-0.0013 (6)	-0.0020 (6)	0.0015 (6)
C7	0.0230 (8)	0.0117 (8)	0.0131 (7)	-0.0015 (6)	-0.0037 (6)	-0.0015 (6)
C8	0.0079 (6)	0.0130 (7)	0.0095 (7)	0.0012 (5)	0.0011 (5)	-0.0006 (6)
N1	0.0120 (6)	0.0118 (6)	0.0101 (6)	-0.0012 (5)	0.0007 (5)	-0.0010 (5)
N2	0.0108 (6)	0.0168 (7)	0.0153 (7)	-0.0009 (5)	0.0021 (5)	0.0002 (5)
C9	0.0120 (7)	0.0138 (7)	0.0126 (7)	-0.0012 (6)	0.0009 (6)	0.0000 (6)
C10	0.0157 (7)	0.0194 (8)	0.0114 (7)	-0.0020 (6)	0.0029 (6)	-0.0007 (6)
C11	0.0153 (7)	0.0173 (8)	0.0105 (7)	-0.0021 (6)	0.0004 (6)	0.0002 (6)
N3	0.0116 (6)	0.0126 (6)	0.0104 (6)	0.0004 (5)	0.0008 (5)	0.0002 (5)
N4	0.0121 (6)	0.0157 (7)	0.0158 (7)	0.0017 (5)	0.0021 (5)	-0.0027 (5)
C12	0.0169 (7)	0.0143 (8)	0.0124 (7)	0.0000 (6)	0.0009 (6)	0.0024 (6)
C13	0.0151 (7)	0.0182 (8)	0.0123 (7)	-0.0036 (6)	0.0023 (6)	0.0010 (6)
C14	0.0127 (7)	0.0118 (7)	0.0135 (7)	0.0002 (6)	-0.0009 (6)	-0.0001 (6)
N5	0.0121 (6)	0.0115 (6)	0.0124 (6)	-0.0016 (5)	0.0011 (5)	-0.0002 (5)
N6	0.0172 (7)	0.0139 (7)	0.0161 (7)	-0.0062 (6)	-0.0014 (5)	0.0019 (5)
C15	0.0156 (7)	0.0131 (7)	0.0135 (7)	-0.0001 (6)	0.0019 (6)	-0.0009 (6)
C16	0.0200 (8)	0.0130 (8)	0.0147 (7)	-0.0010 (6)	-0.0015 (6)	-0.0014 (6)
C17	0.0131 (7)	0.0158 (8)	0.0151 (7)	-0.0023 (6)	0.0008 (6)	-0.0004 (6)

Geometric parameters (Å, °)

Co—O2W	2.1064 (11)	N1—C9	1.3204 (19)
Co—N3	2.1076 (13)	N1—C11	1.3825 (19)
Co—N5	2.1124 (13)	N2—C9	1.345 (2)
Co—N1	2.1347 (13)	N2—C10	1.376 (2)
Co—O1	2.1442 (10)	N2—H2N	0.86 (2)
Co—O1W	2.1680 (11)	C9—H9	0.9500
O1W—H1W	0.85 (3)	C10—C11	1.362 (2)
O1W—H2W	0.85 (3)	C10—H10	0.9500
O2W—H3W	0.82 (3)	C11—H11	0.9500
O2W—H4W	0.82 (2)	N3—C14	1.322 (2)
O3W—H5W	0.81 (2)	N3—C12	1.383 (2)
O3W—H6W	0.82 (3)	N4—C14	1.342 (2)
O1—C1	1.2765 (19)	N4—C13	1.369 (2)
O2—C1	1.2471 (19)	N4—H4N	0.85 (2)
O3—C8	1.2738 (18)	C12—C13	1.356 (2)
O4—C8	1.2450 (19)	C12—H12	0.9500
C1—C2	1.511 (2)	C13—H13	0.9500
C2—C3	1.390 (2)	C14—H14	0.9500
C2—C7	1.393 (2)	N5—C17	1.327 (2)
C3—C4	1.387 (2)	N5—C15	1.380 (2)
C3—H3	0.9500	N6—C17	1.337 (2)
C4—C5	1.395 (2)	N6—C16	1.366 (2)
C4—H4	0.9500	N6—H6N	0.84 (2)
C5—C6	1.391 (2)	C15—C16	1.358 (2)
C5—C8	1.509 (2)	C15—H15	0.9500
C6—C7	1.391 (2)	C16—H16	0.9500

C6—H6	0.9500	C17—H17	0.9500
C7—H7	0.9500		
O2W—Co—N3	90.33 (5)	O3—C8—C5	117.34 (13)
O2W—Co—N5	92.80 (5)	C9—N1—C11	105.60 (13)
N3—Co—N5	93.56 (5)	C9—N1—Co	126.08 (10)
O2W—Co—N1	87.96 (5)	C11—N1—Co	128.17 (10)
N3—Co—N1	175.12 (5)	C9—N2—C10	107.31 (13)
N5—Co—N1	91.09 (5)	C9—N2—H2N	124.9 (15)
O2W—Co—O1	175.14 (5)	C10—N2—H2N	127.3 (15)
N3—Co—O1	91.44 (4)	N1—C9—N2	111.54 (14)
N5—Co—O1	91.60 (5)	N1—C9—H9	124.2
N1—Co—O1	89.91 (5)	N2—C9—H9	124.2
O2W—Co—O1W	87.05 (5)	C11—C10—N2	106.07 (14)
N3—Co—O1W	85.59 (5)	C11—C10—H10	127.0
N5—Co—O1W	179.13 (5)	N2—C10—H10	127.0
N1—Co—O1W	89.76 (5)	C10—C11—N1	109.48 (14)
O1—Co—O1W	88.57 (4)	C10—C11—H11	125.3
Co—O1W—H1W	101.0 (18)	N1—C11—H11	125.3
Co—O1W—H2W	117.2 (16)	C14—N3—C12	105.64 (13)
H1W—O1W—H2W	104 (2)	C14—N3—Co	123.89 (11)
Co—O2W—H3W	120.8 (17)	C12—N3—Co	130.35 (11)
Co—O2W—H4W	124.3 (16)	C14—N4—C13	107.78 (14)
H3W—O2W—H4W	110 (2)	C14—N4—H4N	126.4 (14)
H5W—O3W—H6W	106 (2)	C13—N4—H4N	125.7 (14)
C1—O1—Co	127.94 (10)	C13—C12—N3	109.42 (14)
O2—C1—O1	125.22 (14)	C13—C12—H12	125.3
O2—C1—C2	118.35 (14)	N3—C12—H12	125.3
O1—C1—C2	116.43 (13)	C12—C13—N4	106.11 (14)
C3—C2—C7	119.42 (14)	C12—C13—H13	126.9
C3—C2—C1	120.70 (14)	N4—C13—H13	126.9
C7—C2—C1	119.87 (14)	N3—C14—N4	111.05 (14)
C4—C3—C2	120.44 (14)	N3—C14—H14	124.5
C4—C3—H3	119.8	N4—C14—H14	124.5
C2—C3—H3	119.8	C17—N5—C15	104.94 (13)
C3—C4—C5	120.18 (14)	C17—N5—Co	127.98 (11)
C3—C4—H4	119.9	C15—N5—Co	125.69 (10)
C5—C4—H4	119.9	C17—N6—C16	108.07 (14)
C6—C5—C4	119.39 (14)	C17—N6—H6N	123.5 (15)
C6—C5—C8	120.01 (14)	C16—N6—H6N	128.1 (15)
C4—C5—C8	120.59 (13)	C16—C15—N5	110.03 (14)
C7—C6—C5	120.30 (15)	C16—C15—H15	125.0
C7—C6—H6	119.9	N5—C15—H15	125.0
C5—C6—H6	119.9	C15—C16—N6	105.63 (14)
C6—C7—C2	120.18 (15)	C15—C16—H16	127.2
C6—C7—H7	119.9	N6—C16—H16	127.2
C2—C7—H7	119.9	N5—C17—N6	111.33 (14)
O4—C8—O3	123.78 (14)	N5—C17—H17	124.3

O4—C8—C5

118.87 (13)

N6—C17—H17

124.3

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2N...O1 ⁱ	0.86 (2)	2.09 (2)	2.9204 (17)	162 (2)
N4—H4N...O3W ⁱⁱ	0.85 (2)	2.18 (2)	2.9842 (18)	157.0 (19)
N4—H4N...O4 ⁱⁱⁱ	0.85 (2)	2.50 (2)	2.9521 (18)	114.5 (17)
N6—H6N...O3 ^{iv}	0.84 (2)	2.02 (2)	2.8249 (18)	162 (2)
O1W—H1W...O2	0.85 (3)	1.79 (3)	2.6160 (16)	163 (3)
O1W—H2W...O4 ^v	0.85 (3)	1.85 (3)	2.6606 (16)	161 (2)
O2W—H3W...O3 ^{vi}	0.82 (3)	1.95 (3)	2.7516 (16)	168 (2)
O2W—H4W...O3W ^{vii}	0.82 (2)	2.00 (2)	2.8118 (17)	172 (2)
O3W—H5W...O1W	0.81 (2)	2.08 (2)	2.8632 (16)	164 (2)
O3W—H6W...O3 ^{vi}	0.82 (3)	1.95 (3)	2.7528 (17)	167 (2)

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