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(5-Aminoisophthalato-κN)triaqua(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II) trihydrate

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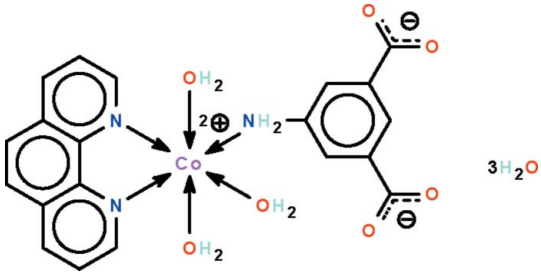
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.086; data-to-parameter ratio = 15.7.

The Co^{II} atom in the title compound, $[Co(C_8H_5NO_4)(C_{12}H_8N_2)(H_2O)_3]\cdot 3H_2O$, is six-coordinated in a CoN_3O_3 octahedral geometry; the water-coordinated Co^{II} atom is chelated by the *N*-heterocycle. An intermolecular N—H···O hydrogen bond occurs. The carboxylate entity coordinates through the amino group. The carboxylate donor unit, coordinated and uncoordinated water molecules interact through O—H···O and N—H···O hydrogen bonds, generating a tightly-held three-dimensional cage-like network.

Related literature

For related structures, see: He *et al.* (2006); Wu *et al.* (2002*a*,*b*).



Experimental

Crystal data

$[Co(C_8H_5NO_4)(C_{12}H_8N_2)(H_2O)_3]\cdot 3H_2O$
M_r = 526.36
Monoclinic, $P2_1/n$
a = 10.1182 (2) Å
b = 13.9659 (2) Å
c = 16.2850 (2) Å
β = 95.827 (1)°
V = 2289.34 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 293 K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.803, T_{max} = 1.000
18954 measured reflections
5683 independent reflections
5120 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.086
S = 1.04
5683 reflections
363 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O6w^{i}	0.83 (1)	1.90 (1)	2.734 (1)	175 (2)
O1w—H1w2···O2^{ii}	0.84 (1)	1.81 (1)	2.646 (1)	173 (2)
O2w—H2w1···O5w^{i}	0.83 (1)	1.93 (1)	2.761 (1)	174 (2)
O2w—H2w2···O4^{iii}	0.85 (1)	1.94 (1)	2.790 (1)	173 (2)
O3w—H3w1···O5w^{iv}	0.84 (1)	2.16 (2)	2.909 (2)	148 (2)
O3w—H3w2···O3^{ii}	0.85 (1)	1.86 (1)	2.694 (1)	167 (2)
O4w—H4w1···O6w^{v}	0.85 (1)	1.98 (1)	2.811 (2)	169 (2)
O4w—H4w2···O2^{iv}	0.85 (1)	2.05 (1)	2.864 (2)	161 (3)
O5w—H5w1···O1	0.85 (1)	1.89 (1)	2.716 (2)	164 (2)
O5w—H5w2···O3^{vi}	0.85 (1)	1.90 (1)	2.719 (1)	161 (2)
O6w—H6w1···O1	0.85 (1)	1.82 (1)	2.665 (1)	174 (2)
O6w—H6w2···O4^{iii}	0.85 (1)	1.94 (1)	2.784 (1)	174 (2)
N1—H1*N*1···O4w	0.85 (1)	2.06 (1)	2.906 (2)	169 (2)
N1—H1*N*2···O4^{iii}	0.84 (1)	2.30 (1)	3.110 (2)	161 (2)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x-1, y, z$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2299).

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supporting information

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(5-Aminoisophthalato-κN)triaqua(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II) trihydrate

Kou-Lin Zhang, Guo-Wang Diao and Seik Weng Ng

S1. Comment

The dianion of 5-aminoisophthalic acid binds to cobalt(II) in a bridging μ_4-manner in the monoaqua derivative (Wu *et al.*, 2002*a*), and the carboxyl oxygen as well as the amino nitrogen atoms are all involved in bonding in the three-dimensional network structure. A diaqua dihydrate has also been reported; the compound has the monoanion in μ_2 bridging that gives rise to a chain motif (Wu *et al.*, 2002*b*). The 4,4′-bipyridine spacer ligand lowers the dimensionality of cobalt 5-amino-isophthalate, and the diqua adduct, which crystallizes as a DMF solvate, exists as linear chains (He *et al.*, 2006). The present 1,10-phenanthroline adduct is a triaqua trihydrate (Scheme I) in which the 5-aminosophthlate dianion binds only through the neutral amino donor site; the coordinated water molecules comprise the *fac* points of the octahedron around the metal atom (Fig. 1). The zwitterionic dianion, the coordinated and lattice water molecules interact through hydrogen bonds (Table 2) to furnish a tightly-held, three-dimensional network. Pairs of phenanthroline units show $\pi\cdots\pi$ interactions about a center-of-inversion at a distance of *ca* 3.5 Å (Fig. 2).

S2. Experimental

Cobalt(II) nitrate hexahydrate (0.048 g, 0.165 mmol) dissolved in water (5 ml) was added to a mixture of 5-amino-isophthalic acid (0.030 g, 0.165 mmol) and sodium hydroxidie (0.013 g, 0.330 mmol) dissolved in water (5 ml). To this solution was added 1,10-phenanthroline (0.033 g, 0.165 mmol) dissolved in methanol (10 ml). The mixture was filtered and set aside for the growth of deep red crystals (35% yield based on the acid). CHN elemental analaysis. Calc. for $C_{20}H_{25}C_{O}N_3O_{10}$: C 45.63, H 4.79, N 7.98%. Found: C, 45.49; H, 4.89; N,7.91%.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The amino and water bound H-atoms were located in difference Fourier maps, and were refined with a distance restraint of N–H = O–H = 0.85±0.01 Å. Their temperature factors were freely refined.

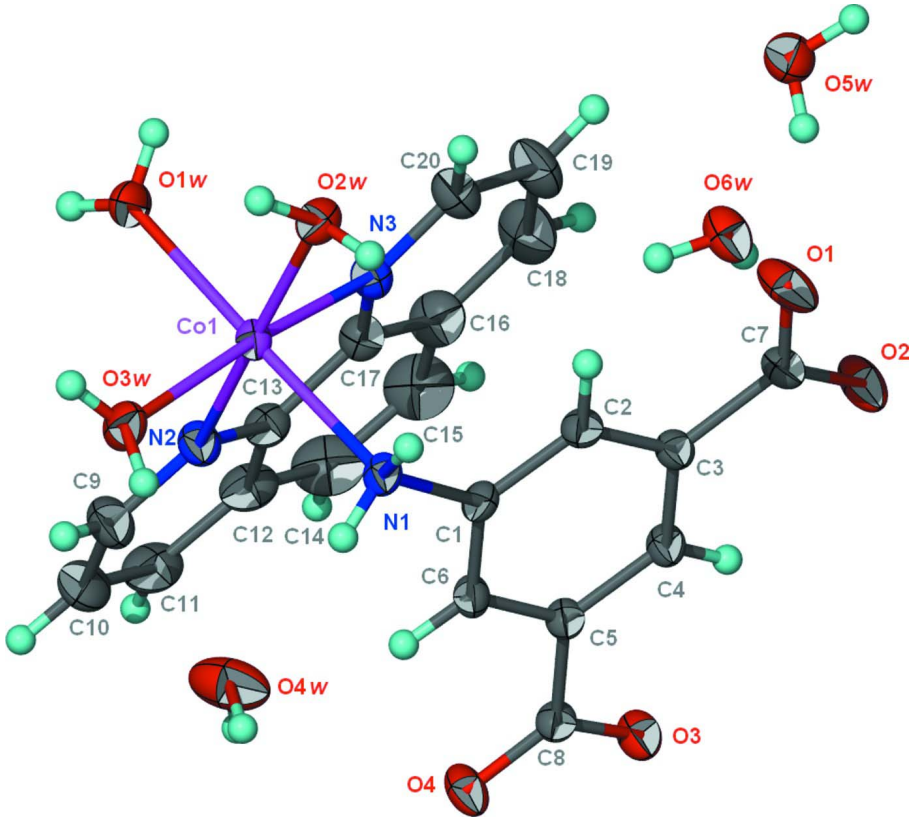

Figure 1

Thermal displacement ellipsoid plot of (I) at the 70% probability level; hydrogen atoms are shown as spheres of arbitrary radii.

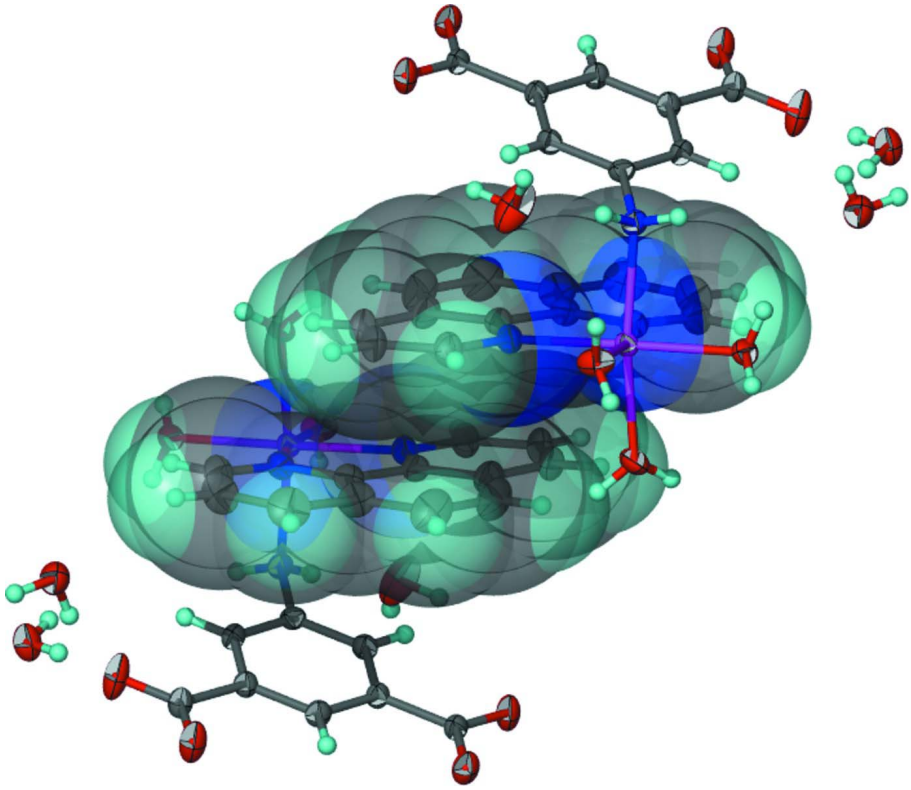

Figure 2

Two formula units of (I) showing $\pi\cdots\pi$ interactions about a center-of-inversion.

(5-Aminoisophthalato-κN)triaqua(1,10-phenanthroline-κ^2N,N')cobalt(II) trihydrate

Crystal data

$[Co(C_8H_5NO_4)(C_{12}H_8N_2)(H_2O)_3]\cdot 3H_2O$
$M_r = 526.36$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.1182\ (2)$ Å
$b = 13.9659\ (2)$ Å
$c = 16.2850\ (2)$ Å
$\beta = 95.827\ (1)°$
$V = 2289.34\ (8)$ Å^3
$Z = 4$
$F(000) = 1092$
$D_x = 1.527$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9790 reflections
$\theta = 2.5–28.5°$
$\mu = 0.81$ mm^{-1}
$T = 293$ K
Prism, red
0.24 × 0.22 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.803$, $T_{max} = 1.000$
18954 measured reflections
5683 independent reflections
5120 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.5°$
$h = -13\rightarrow13$
$k = -18\rightarrow18$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.086$
$S = 1.04$
5683 reflections
363 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.5451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.742889 (15)	0.684399 (12)	0.466367 (10)	0.01480 (6)
O1	1.15673 (10)	0.53092 (8)	0.26398 (8)	0.0313 (2)
O2	1.22644 (9)	0.64316 (8)	0.18340 (7)	0.0283 (2)
O3	0.92170 (9)	0.91482 (7)	0.09694 (6)	0.02231 (19)
O4	0.72213 (9)	0.92307 (7)	0.14075 (6)	0.0237 (2)
O1W	0.76586 (10)	0.70374 (8)	0.59335 (6)	0.0228 (2)
H1W1	0.8296 (15)	0.6766 (13)	0.6202 (12)	0.036 (6)*
H1W2	0.749 (2)	0.7538 (11)	0.6187 (13)	0.052 (7)*
O2W	0.79629 (9)	0.54265 (7)	0.49718 (6)	0.01971 (18)
H2W1	0.7468 (16)	0.5247 (15)	0.5321 (10)	0.037 (6)*
H2W2	0.784 (2)	0.5056 (14)	0.4555 (10)	0.049 (6)*
O3W	0.53714 (9)	0.66780 (8)	0.47286 (6)	0.0235 (2)
H3W1	0.486 (2)	0.6450 (17)	0.4334 (11)	0.057 (7)*
H3W2	0.509 (2)	0.6474 (15)	0.5168 (9)	0.042 (6)*
O4W	0.44314 (12)	0.71848 (11)	0.29095 (9)	0.0424 (3)
H4W1	0.451 (2)	0.7710 (11)	0.2661 (14)	0.056 (7)*
H4W2	0.390 (2)	0.6844 (17)	0.2600 (15)	0.067 (9)*
O5W	1.35918 (11)	0.52866 (8)	0.38701 (7)	0.0276 (2)
H5W1	1.3070 (18)	0.5252 (16)	0.3431 (9)	0.041 (6)*
H5W2	1.4231 (15)	0.4911 (13)	0.3801 (13)	0.040 (6)*
O6W	1.02652 (9)	0.37775 (7)	0.31095 (7)	0.0248 (2)
H6W1	1.063 (2)	0.4287 (10)	0.2960 (13)	0.044 (6)*
H6W2	0.9517 (13)	0.3885 (15)	0.3285 (13)	0.045 (6)*
N1	0.70534 (10)	0.63853 (8)	0.33691 (6)	0.0168 (2)
H1N1	0.6259 (11)	0.6547 (13)	0.3202 (11)	0.023 (4)*
H1N2	0.7054 (19)	0.5782 (7)	0.3384 (12)	0.031 (5)*
N2	0.71726 (11)	0.83333 (8)	0.43935 (7)	0.0198 (2)
N3	0.94173 (10)	0.73017 (8)	0.45306 (7)	0.0186 (2)
C1	0.79644 (12)	0.67271 (9)	0.28227 (7)	0.0155 (2)
C2	0.91651 (12)	0.62476 (9)	0.27734 (7)	0.0166 (2)
H2	0.9344	0.5688	0.3074	0.020*
C3	1.00960 (11)	0.66020 (9)	0.22771 (7)	0.0160 (2)
C4	0.98255 (12)	0.74438 (9)	0.18275 (8)	0.0170 (2)

H4	1.0446	0.7686	0.1498	0.020*
C5	0.86219 (11)	0.79214 (9)	0.18732 (7)	0.0158 (2)
C6	0.76966 (12)	0.75642 (9)	0.23778 (7)	0.0168 (2)
H6	0.6902	0.7888	0.2415	0.020*
C7	1.14016 (11)	0.60753 (9)	0.22423 (8)	0.0180 (2)
C8	0.83353 (12)	0.88295 (9)	0.13858 (7)	0.0164 (2)
C9	0.60574 (14)	0.88414 (11)	0.43592 (9)	0.0264 (3)
H9	0.5278	0.8534	0.4466	0.032*
C10	0.60072 (16)	0.98217 (12)	0.41679 (10)	0.0316 (3)
H10	0.5210	1.0156	0.4157	0.038*
C11	0.71446 (17)	1.02817 (11)	0.39974 (9)	0.0307 (3)
H11	0.7127	1.0932	0.3875	0.037*
C12	0.83406 (15)	0.97630 (10)	0.40083 (9)	0.0259 (3)
C13	0.83020 (13)	0.87881 (10)	0.42259 (8)	0.0195 (2)
C14	0.95735 (17)	1.01683 (12)	0.38069 (11)	0.0365 (4)
H14	0.9602	1.0810	0.3657	0.044*
C15	1.06906 (17)	0.96363 (13)	0.38306 (12)	0.0379 (4)
H15	1.1469	0.9912	0.3682	0.045*
C16	1.06940 (14)	0.86486 (12)	0.40818 (10)	0.0280 (3)
C17	0.95058 (13)	0.82265 (10)	0.42820 (8)	0.0198 (2)
C18	1.18338 (15)	0.80580 (13)	0.41512 (11)	0.0353 (4)
H18	1.2640	0.8297	0.4013	0.042*
C19	1.17504 (14)	0.71351 (13)	0.44210 (11)	0.0326 (3)
H19	1.2503	0.6749	0.4482	0.039*
C20	1.05169 (13)	0.67760 (10)	0.46052 (9)	0.0245 (3)
H20	1.0469	0.6147	0.4786	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01501 (9)	0.01376 (10)	0.01610 (10)	0.00058 (5)	0.00396 (6)	0.00020 (6)
O1	0.0198 (4)	0.0260 (5)	0.0490 (7)	0.0059 (4)	0.0081 (4)	0.0196 (5)
O2	0.0216 (4)	0.0249 (5)	0.0407 (6)	0.0061 (4)	0.0137 (4)	0.0139 (5)
O3	0.0215 (4)	0.0204 (5)	0.0265 (5)	0.0018 (4)	0.0095 (3)	0.0082 (4)
O4	0.0216 (4)	0.0192 (5)	0.0320 (5)	0.0066 (4)	0.0109 (4)	0.0087 (4)
O1W	0.0260 (5)	0.0237 (5)	0.0185 (4)	0.0059 (4)	0.0009 (4)	−0.0061 (4)
O2W	0.0266 (4)	0.0146 (4)	0.0182 (4)	−0.0006 (4)	0.0031 (3)	−0.0010 (4)
O3W	0.0170 (4)	0.0344 (5)	0.0198 (5)	−0.0033 (4)	0.0045 (3)	−0.0009 (4)
O4W	0.0265 (5)	0.0461 (8)	0.0526 (8)	−0.0063 (5)	−0.0051 (5)	0.0224 (7)
O5W	0.0306 (5)	0.0256 (5)	0.0269 (5)	0.0060 (4)	0.0045 (4)	0.0030 (4)
O6W	0.0206 (4)	0.0192 (5)	0.0354 (5)	0.0003 (4)	0.0073 (4)	0.0018 (4)
N1	0.0181 (4)	0.0166 (5)	0.0165 (5)	−0.0001 (4)	0.0058 (4)	0.0032 (4)
N2	0.0202 (5)	0.0180 (5)	0.0214 (5)	0.0022 (4)	0.0036 (4)	0.0007 (4)
N3	0.0171 (5)	0.0184 (5)	0.0205 (5)	−0.0001 (4)	0.0025 (4)	−0.0015 (4)
C1	0.0175 (5)	0.0165 (5)	0.0132 (5)	−0.0008 (4)	0.0041 (4)	0.0009 (4)
C2	0.0192 (5)	0.0147 (5)	0.0161 (5)	0.0009 (4)	0.0024 (4)	0.0027 (4)
C3	0.0157 (5)	0.0152 (5)	0.0172 (5)	0.0011 (4)	0.0022 (4)	0.0005 (4)
C4	0.0171 (5)	0.0167 (6)	0.0180 (5)	0.0000 (4)	0.0051 (4)	0.0024 (5)

C5	0.0175 (5)	0.0139 (5)	0.0166 (5)	0.0008 (4)	0.0041 (4)	0.0022 (4)
C6	0.0168 (5)	0.0172 (6)	0.0171 (5)	0.0020 (4)	0.0051 (4)	0.0006 (5)
C7	0.0152 (5)	0.0166 (6)	0.0222 (6)	0.0011 (4)	0.0020 (4)	0.0028 (5)
C8	0.0194 (5)	0.0136 (5)	0.0164 (5)	0.0008 (4)	0.0035 (4)	0.0018 (4)
C9	0.0251 (6)	0.0243 (7)	0.0308 (7)	0.0063 (5)	0.0066 (5)	0.0030 (6)
C10	0.0378 (8)	0.0258 (7)	0.0313 (7)	0.0149 (6)	0.0044 (6)	0.0046 (6)
C11	0.0465 (8)	0.0180 (6)	0.0267 (7)	0.0059 (6)	−0.0005 (6)	0.0034 (6)
C12	0.0349 (7)	0.0185 (6)	0.0236 (6)	−0.0026 (5)	−0.0004 (5)	0.0037 (5)
C13	0.0234 (6)	0.0172 (6)	0.0178 (5)	−0.0011 (5)	0.0019 (4)	0.0006 (5)
C14	0.0441 (9)	0.0232 (7)	0.0416 (9)	−0.0111 (6)	0.0012 (7)	0.0102 (7)
C15	0.0344 (8)	0.0343 (9)	0.0454 (9)	−0.0156 (7)	0.0063 (7)	0.0089 (7)
C16	0.0239 (6)	0.0296 (7)	0.0309 (7)	−0.0085 (6)	0.0050 (5)	0.0024 (6)
C17	0.0196 (6)	0.0199 (6)	0.0201 (6)	−0.0025 (5)	0.0026 (4)	−0.0012 (5)
C18	0.0186 (6)	0.0439 (10)	0.0441 (9)	−0.0075 (6)	0.0068 (6)	−0.0006 (7)
C19	0.0166 (6)	0.0376 (8)	0.0436 (9)	0.0031 (6)	0.0034 (6)	−0.0033 (7)
C20	0.0202 (6)	0.0229 (7)	0.0302 (7)	0.0027 (5)	0.0011 (5)	−0.0025 (5)

Geometric parameters (Å, º)

Co1—O1W	2.0750 (10)	C1—C2	1.3967 (16)
Co1—O2W	2.0995 (9)	C2—C3	1.3927 (16)
Co1—O3W	2.1080 (9)	C2—H2	0.9300
Co1—N2	2.1364 (12)	C3—C4	1.3974 (17)
Co1—N3	2.1429 (10)	C3—C7	1.5181 (16)
Co1—N1	2.1992 (11)	C4—C5	1.3971 (16)
O1—C7	1.2530 (16)	C4—H4	0.9300
O2—C7	1.2530 (15)	C5—C6	1.3989 (16)
O3—C8	1.2556 (14)	C5—C8	1.5086 (17)
O4—C8	1.2624 (15)	C6—H6	0.9300
O1W—H1W1	0.83 (1)	C9—C10	1.404 (2)
O1W—H1W2	0.84 (1)	C9—H9	0.9300
O2W—H2W1	0.83 (1)	C10—C11	1.371 (2)
O2W—H2W2	0.85 (1)	C10—H10	0.9300
O3W—H3W1	0.84 (1)	C11—C12	1.409 (2)
O3W—H3W2	0.85 (1)	C11—H11	0.9300
O4W—H4W1	0.85 (1)	C12—C13	1.4085 (19)
O4W—H4W2	0.85 (1)	C12—C14	1.438 (2)
O5W—H5W1	0.85 (1)	C13—C17	1.4437 (18)
O5W—H5W2	0.85 (1)	C14—C15	1.350 (3)
O6W—H6W1	0.85 (1)	C14—H14	0.9300
O6W—H6W2	0.85 (1)	C15—C16	1.439 (2)
N1—C1	1.4269 (15)	C15—H15	0.9300
N1—H1N1	0.85 (1)	C16—C17	1.4066 (18)
N1—H1N2	0.84 (1)	C16—C18	1.413 (2)
N2—C9	1.3293 (17)	C18—C19	1.367 (2)
N2—C13	1.3590 (17)	C18—H18	0.9300
N3—C20	1.3282 (17)	C19—C20	1.405 (2)
N3—C17	1.3593 (17)	C19—H19	0.9300

C1—C6	1.3876 (17)	C20—H20	0.9300
O1W—Co1—O2W	83.37 (4)	C3—C4—H4	120.0
O1W—Co1—O3W	88.60 (4)	C4—C5—C6	120.00 (11)
O2W—Co1—O3W	96.65 (4)	C4—C5—C8	119.70 (10)
O1W—Co1—N2	94.45 (4)	C6—C5—C8	120.29 (11)
O2W—Co1—N2	171.97 (4)	C1—C6—C5	120.02 (11)
O3W—Co1—N2	91.01 (4)	C1—C6—H6	120.0
O1W—Co1—N3	92.90 (4)	C5—C6—H6	120.0
O2W—Co1—N3	94.82 (4)	O2—C7—O1	123.33 (11)
O3W—Co1—N3	168.53 (4)	O2—C7—C3	118.90 (11)
N2—Co1—N3	77.54 (4)	O1—C7—C3	117.76 (11)
O1W—Co1—N1	169.81 (4)	O3—C8—O4	122.90 (11)
O2W—Co1—N1	88.26 (4)	O3—C8—C5	118.22 (11)
O3W—Co1—N1	86.60 (4)	O4—C8—C5	118.88 (10)
N2—Co1—N1	94.62 (4)	N2—C9—C10	122.77 (14)
N3—Co1—N1	93.59 (4)	N2—C9—H9	118.6
Co1—O1W—H1W1	117.8 (15)	C10—C9—H9	118.6
Co1—O1W—H1W2	126.2 (16)	C11—C10—C9	119.33 (14)
H1W1—O1W—H1W2	108 (2)	C11—C10—H10	120.3
Co1—O2W—H2W1	106.8 (15)	C9—C10—H10	120.3
Co1—O2W—H2W2	111.5 (16)	C10—C11—C12	119.61 (14)
H2W1—O2W—H2W2	108 (2)	C10—C11—H11	120.2
Co1—O3W—H3W1	122.1 (17)	C12—C11—H11	120.2
Co1—O3W—H3W2	120.1 (15)	C13—C12—C11	117.03 (13)
H3W1—O3W—H3W2	106 (2)	C13—C12—C14	119.00 (14)
H4W1—O4W—H4W2	107 (2)	C11—C12—C14	123.96 (14)
H5W1—O5W—H5W2	106 (2)	N2—C13—C12	123.20 (12)
H6W1—O6W—H6W2	112 (2)	N2—C13—C17	117.04 (12)
C1—N1—Co1	116.15 (8)	C12—C13—C17	119.75 (12)
C1—N1—H1N1	111.1 (12)	C15—C14—C12	121.35 (14)
Co1—N1—H1N1	107.1 (12)	C15—C14—H14	119.3
C1—N1—H1N2	110.7 (13)	C12—C14—H14	119.3
Co1—N1—H1N2	105.3 (13)	C14—C15—C16	120.90 (14)
H1N1—N1—H1N2	105.8 (18)	C14—C15—H15	119.5
C9—N2—C13	118.01 (12)	C16—C15—H15	119.5
C9—N2—Co1	127.81 (10)	C17—C16—C18	116.54 (14)
C13—N2—Co1	114.17 (9)	C17—C16—C15	119.36 (14)
C20—N3—C17	118.20 (11)	C18—C16—C15	124.11 (14)
C20—N3—Co1	127.75 (10)	N3—C17—C16	123.43 (13)
C17—N3—Co1	113.86 (8)	N3—C17—C13	117.02 (11)
C6—C1—C2	119.92 (11)	C16—C17—C13	119.55 (13)
C6—C1—N1	120.22 (11)	C19—C18—C16	119.97 (14)
C2—C1—N1	119.75 (11)	C19—C18—H18	120.0
C3—C2—C1	120.43 (11)	C16—C18—H18	120.0
C3—C2—H2	119.8	C18—C19—C20	119.35 (14)
C1—C2—H2	119.8	C18—C19—H19	120.3
C2—C3—C4	119.67 (11)	C20—C19—H19	120.3

C2—C3—C7	119.46 (11)	N3—C20—C19	122.48 (14)
C4—C3—C7	120.86 (11)	N3—C20—H20	118.8
C5—C4—C3	119.95 (11)	C19—C20—H20	118.8
C5—C4—H4	120.0		

O1W—Co1—N1—C1	−145.0 (2)	C4—C5—C8—O3	−2.25 (18)
O2W—Co1—N1—C1	−110.28 (9)	C6—C5—C8—O3	176.88 (12)
O3W—Co1—N1—C1	152.95 (9)	C4—C5—C8—O4	177.14 (12)
N2—Co1—N1—C1	62.21 (9)	C6—C5—C8—O4	−3.73 (18)
N3—Co1—N1—C1	−15.56 (9)	C13—N2—C9—C10	−0.8 (2)
O1W—Co1—N2—C9	−85.16 (12)	Co1—N2—C9—C10	−179.49 (11)
O3W—Co1—N2—C9	3.51 (12)	N2—C9—C10—C11	0.9 (2)
N3—Co1—N2—C9	−177.16 (13)	C9—C10—C11—C12	0.7 (2)
N1—Co1—N2—C9	90.18 (12)	C10—C11—C12—C13	−2.1 (2)
O1W—Co1—N2—C13	96.06 (9)	C10—C11—C12—C14	177.43 (16)
O3W—Co1—N2—C13	−175.26 (9)	C9—N2—C13—C12	−0.9 (2)
N3—Co1—N2—C13	4.07 (9)	Co1—N2—C13—C12	178.02 (10)
N1—Co1—N2—C13	−88.59 (9)	C9—N2—C13—C17	178.87 (12)
O1W—Co1—N3—C20	85.77 (12)	Co1—N2—C13—C17	−2.23 (15)
O2W—Co1—N3—C20	2.19 (12)	C11—C12—C13—N2	2.3 (2)
O3W—Co1—N3—C20	−176.94 (17)	C14—C12—C13—N2	−177.27 (14)
N2—Co1—N3—C20	179.69 (12)	C11—C12—C13—C17	−177.44 (13)
N1—Co1—N3—C20	−86.36 (12)	C14—C12—C13—C17	3.0 (2)
O1W—Co1—N3—C17	−99.37 (9)	C13—C12—C14—C15	−0.7 (2)
O2W—Co1—N3—C17	177.06 (9)	C11—C12—C14—C15	179.79 (16)
O3W—Co1—N3—C17	−2.1 (3)	C12—C14—C15—C16	−1.8 (3)
N2—Co1—N3—C17	−5.45 (9)	C14—C15—C16—C17	1.9 (3)
N1—Co1—N3—C17	88.50 (9)	C14—C15—C16—C18	−177.55 (17)
Co1—N1—C1—C6	−92.87 (12)	C20—N3—C17—C16	1.5 (2)
Co1—N1—C1—C2	83.33 (13)	Co1—N3—C17—C16	−173.89 (11)
C6—C1—C2—C3	−0.27 (19)	C20—N3—C17—C13	−178.51 (12)
N1—C1—C2—C3	−176.48 (11)	Co1—N3—C17—C13	6.10 (15)
C1—C2—C3—C4	0.13 (19)	C18—C16—C17—N3	−0.1 (2)
C1—C2—C3—C7	179.20 (11)	C15—C16—C17—N3	−179.52 (14)
C2—C3—C4—C5	−0.45 (19)	C18—C16—C17—C13	179.94 (14)
C7—C3—C4—C5	−179.51 (11)	C15—C16—C17—C13	0.5 (2)
C3—C4—C5—C6	0.91 (19)	N2—C13—C17—N3	−2.64 (18)
C3—C4—C5—C8	−179.95 (11)	C12—C13—C17—N3	177.12 (12)
C2—C1—C6—C5	0.73 (19)	N2—C13—C17—C16	177.35 (12)
N1—C1—C6—C5	176.92 (11)	C12—C13—C17—C16	−2.9 (2)
C4—C5—C6—C1	−1.06 (19)	C17—C16—C18—C19	−1.6 (2)
C8—C5—C6—C1	179.81 (11)	C15—C16—C18—C19	177.86 (17)
C2—C3—C7—O2	−175.69 (12)	C16—C18—C19—C20	1.7 (3)
C4—C3—C7—O2	3.38 (19)	C17—N3—C20—C19	−1.3 (2)
C2—C3—C7—O1	3.05 (18)	Co1—N3—C20—C19	173.33 (11)
C4—C3—C7—O1	−177.88 (13)	C18—C19—C20—N3	−0.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O6w^{i}	0.83 (1)	1.90 (1)	2.734 (1)	175 (2)
O1w—H1w2···O2^{ii}	0.84 (1)	1.81 (1)	2.646 (1)	173 (2)
O2w—H2w1···O5w^{i}	0.83 (1)	1.93 (1)	2.761 (1)	174 (2)
O2w—H2w2···O4^{iii}	0.85 (1)	1.94 (1)	2.790 (1)	173 (2)
O3w—H3w1···O5w^{iv}	0.84 (1)	2.16 (2)	2.909 (2)	148 (2)
O3w—H3w2···O3^{ii}	0.85 (1)	1.86 (1)	2.694 (1)	167 (2)
O4w—H4w1···O6w^{v}	0.85 (1)	1.98 (1)	2.811 (2)	169 (2)
O4w—H4w2···O2^{iv}	0.85 (1)	2.05 (1)	2.864 (2)	161 (3)
O5w—H5w1···O1	0.85 (1)	1.89 (1)	2.716 (2)	164 (2)
O5w—H5w2···O3^{vi}	0.85 (1)	1.90 (1)	2.719 (1)	161 (2)
O6w—H6w1···O1	0.85 (1)	1.82 (1)	2.665 (1)	174 (2)
O6w—H6w2···O4^{iii}	0.85 (1)	1.94 (1)	2.784 (1)	174 (2)
N1—H1*N*1···O4w	0.85 (1)	2.06 (1)	2.906 (2)	169 (2)
N1—H1*N*2···O4^{iii}	0.84 (1)	2.30 (1)	3.110 (2)	161 (2)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*−1/2, −*y*+3/2, *z*+1/2; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*; (v) −*x*+3/2, *y*+1/2, −*z*+1/2; (vi) −*x*+5/2, *y*−1/2, −*z*+1/2.