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Bis[1,3-bis(benzimidazol-2-yl)-2-oxapropane]cobalt(II) dipicrate acetonitrile trisolvate

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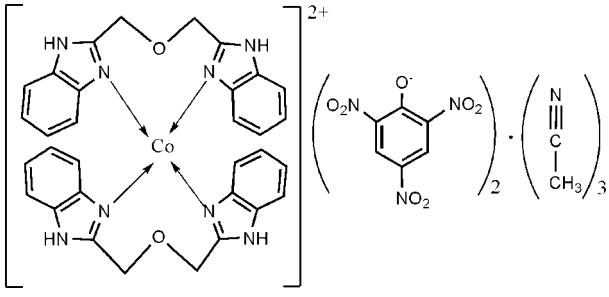
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.087; data-to-parameter ratio = 15.5.

In the title compound, $[Co(C_{16}H_{14}N_4O)_2](C_6H_2N_3O_7)_2\cdot 3CH_3CN$, the Co^{II} ion is located on a crystallographic twofold rotation axis and is coordinated in a slightly distorted tetrahedral environment by four N atoms from the two bidentate *N*-heterocycles. The crystal structure is stabilized by intermolecular N—H···O and N—H···N hydrogen bonds. One of the acetonitrile solvent molecules also lies on a twofold rotation axis.

Related literature

For the crystal structures of related dipicrate metal complexes with 1,3-bis(1-benzyl-1H-benzimidazol-2-yl)-2-oxapropane ligands, see: Wu, Yun, Li, Wang & Huang (2009); Wu, Yun, Li, Tao & Wang (2009).



Experimental

Crystal data

$[Co(C_{16}H_{14}N_4O)_2](C_6H_2N_3O_7)_2\cdot 3C_2H_3N$
M_r = 1194.93
Monoclinic, $P2/c$
a = 11.4114 (3) Å
b = 9.9303 (2) Å
c = 25.1442 (6) Å
β = 111.164 (1)°
V = 2657.12 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 153 K
0.28 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.894, T_{max} = 0.933
25278 measured reflections
6093 independent reflections
5418 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.087
S = 1.04
6093 reflections
392 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···O6^{i}	0.858 (9)	1.893 (12)	2.6746 (14)	150.7 (17)
N2—H2*N*···O5^{i}	0.858 (9)	2.381 (15)	3.0166 (15)	131.3 (15)
N4—H4*N*···N8	0.858 (9)	2.052 (10)	2.9040 (18)	171.8 (18)

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: LH2846).

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Wu, H., Yun, R., Li, K., Tao, S. & Wang, K. (2009). *Acta Cryst.* E**65**, m786.
Wu, H., Yun, R., Li, K., Wang, K. & Huang, X. (2009). *Acta Cryst.* E**65**, m751–m752.

supporting information

Acta Cryst. (2009). E**65**, m851 [doi:10.1107/S1600536809024234]

Bis[1,3-bis(benzimidazol-2-yl)-2-oxapropane]cobalt(II) dipicrate acetonitrile trisolvate

Huilu Wu, Ruirui Yun, Xingcai Huang, Qingyu Sun and Baoliang Qi

S1. Comment

The asymmetric unit of the title compound consists of half a discrete di[1,3-bis(benzimidazol-2-yl)-2-oxopropane] cobalt(II) cation, one picrate anion and 1.5 molecules of acetonitrile; the formula unit is generated by a twofold rotation axis. The cation is shown in Fig. 1. The Co^{II} ion is four-coordinate with a N_4 ligand set. The (1,3-bis(benzimidazol-2-yl)-2-oxopropane) ligand acts as a bidentate donor. The coordination geometry of the Co^{II} may be best described as slightly distorted tetrahedral. This geometry is assumed by the Co^{II} to relieve the steric crowding. The crystal structure is stabilized by intermolecular N—H···O and N—H···N hydrogen bonds. Additional stabilization is provided by weak intermolecular C-H···O hydrogen bonds (Fig. 2).

S2. Experimental

To a stirred solution of 1,3-bis(benzimidazol-2-yl)-2-oxopropane (0.139 g, 0.5 mmol) in hot MeOH (15 ml) was added $Co(C_6H_2N_3O_7)_2$ (0.129 g, 0.25 mmol) in MeOH (5 ml). A red crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute Et_2O, and dried *in vacuo*. The dried precipitate was dissolved in acetonitrile to form a red solution that was allowed to evaporate at room temperature. Red crystals suitable for X-ray diffraction studies were obtained after three days at room temperature. Yield, 0.106 g (66%). (found: C, 50.20; H, 3.51; N,19.94. Calcd. for C50H41N17O16Co: C, 50.26; H, 3.46; N, 19.93)

S3. Refinement

All H atoms were found in difference electron maps and were subsequently included in a riding-model approximation with C—H distances ranging from 0.95 to 0.99 Å and U_{iso}(H) = 1.2 U_{eq} of the carrier atom. The H atoms bonded to N atoms were refined independently with the distance constraint of N—H 0.858 (9) Å.

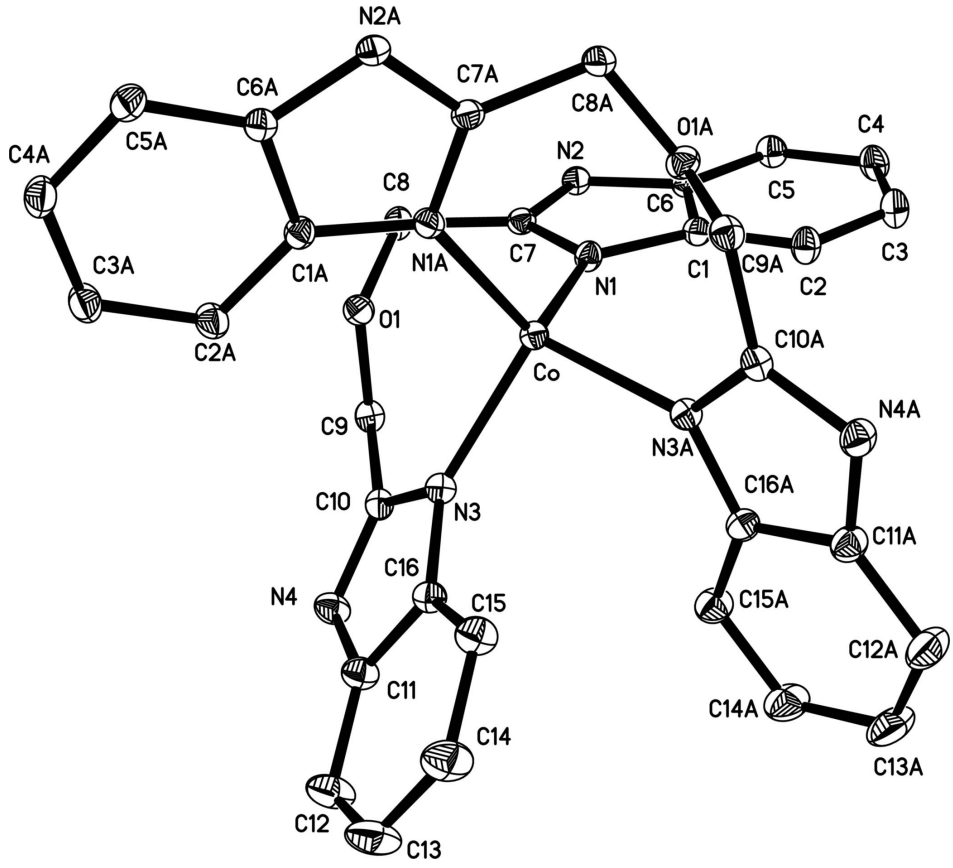

Figure 1

Molecular structure and atom numbering for the cation of the title compound. Hydrogen atoms have been omitted for clarity and the displacement ellipsoids are shown at the 30% probability level [symmetry code: (A) -x+1, y, -z+3/2].

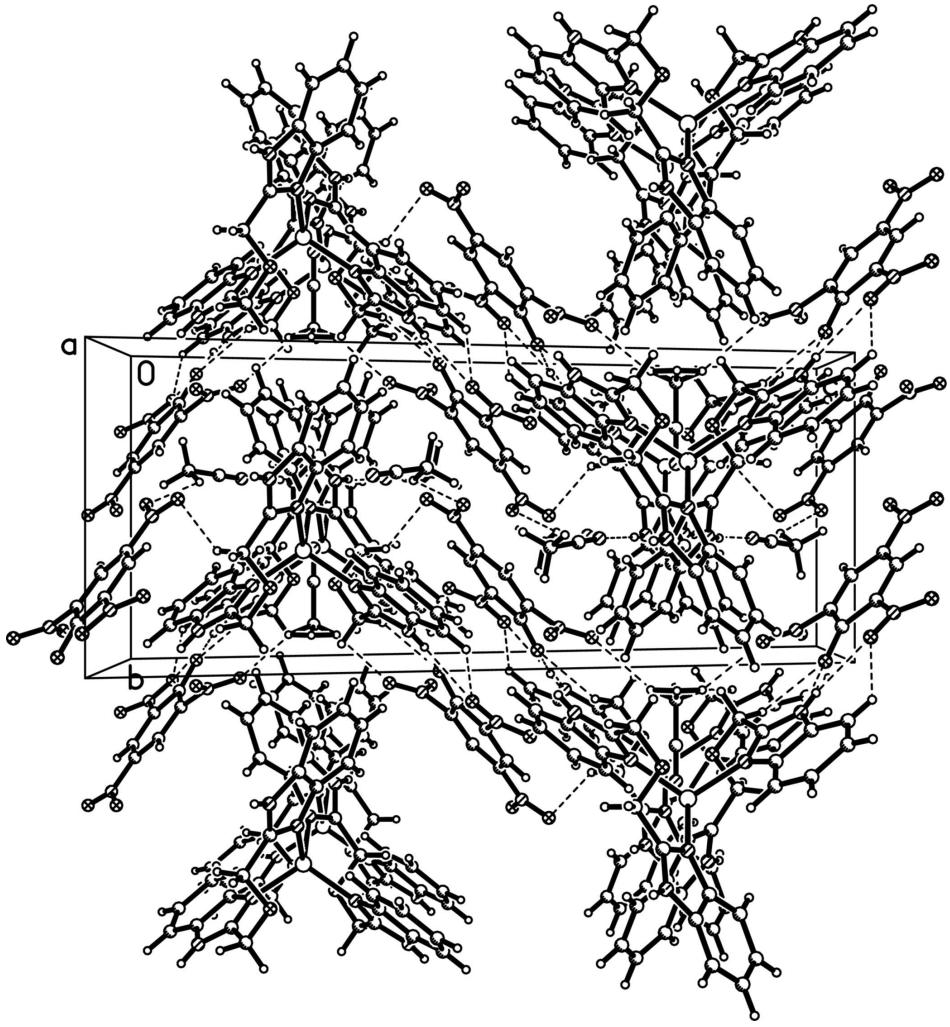

Figure 2

Part of the crystal structure with hydrogen bonds shown as dashed lines.

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Crystal data

$[Co(C_{16}H_{14}N_4O)_2](C_6H_2N_3O_7)_2\cdot 3C_2H_3N$
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Monoclinic, $P2/c$
Hall symbol: -P 2yc
$a = 11.4114\ (3)$ Å
$b = 9.9303\ (2)$ Å
$c = 25.1442\ (6)$ Å
$\beta = 111.164\ (1)°$
$V = 2657.12\ (11)$ Å^3
$Z = 2$
$F(000) = 1230$
$D_x = 1.494$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7749 reflections
$\theta = 3.2–27.5°$
$\mu = 0.41$ mm^{-1}
$T = 153$ K
Block, red
0.28 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.894, T_{max} = 0.933
25278 measured reflections
6093 independent reflections
5418 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −14→14
k = −12→12
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.087
S = 1.04
6093 reflections
392 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.9118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0036 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co	0.5000	0.36301 (2)	0.7500	0.01700 (8)	
O1	0.67337 (8)	0.24981 (9)	0.71220 (4)	0.02259 (19)	
O2	0.74591 (13)	0.49084 (15)	0.46620 (6)	0.0583 (4)	
O3	0.54824 (12)	0.47322 (11)	0.41556 (5)	0.0409 (3)	
O4	0.25535 (11)	0.76959 (16)	0.44436 (6)	0.0567 (4)	
O5	0.29928 (11)	0.88294 (12)	0.52194 (5)	0.0428 (3)	
O6	0.54003 (9)	0.96666 (10)	0.56756 (4)	0.0292 (2)	
O7	0.78254 (12)	0.91568 (16)	0.63960 (5)	0.0522 (3)	
O8	0.88585 (11)	0.89860 (13)	0.58266 (5)	0.0420 (3)	
N1	0.41234 (10)	0.25020 (10)	0.67914 (4)	0.0200 (2)	
N2	0.39034 (10)	0.10735 (11)	0.60795 (4)	0.0202 (2)	
N3	0.62918 (10)	0.49981 (11)	0.74562 (4)	0.0195 (2)	
N4	0.77113 (11)	0.58828 (12)	0.71442 (5)	0.0260 (2)	
N5	0.63674 (13)	0.52737 (13)	0.45326 (5)	0.0342 (3)	
N6	0.33090 (11)	0.81256 (13)	0.48951 (5)	0.0309 (3)	

N7	0.79113 (12)	0.88240 (13)	0.59422 (5)	0.0332 (3)	
N8	0.93174 (15)	0.59702 (16)	0.64743 (6)	0.0452 (4)	
N9	1.0000	0.3626 (2)	0.7500	0.0471 (5)	
C1	0.28403 (12)	0.23999 (12)	0.64561 (5)	0.0196 (2)	
C2	0.17845 (12)	0.29913 (14)	0.65151 (5)	0.0252 (3)	
H2	0.1860	0.3604	0.6816	0.030*	
C3	0.06220 (13)	0.26482 (15)	0.61173 (6)	0.0282 (3)	
H3	−0.0113	0.3029	0.6150	0.034*	
C4	0.04975 (13)	0.17528 (15)	0.56674 (6)	0.0278 (3)	
H4	−0.0317	0.1546	0.5402	0.033*	
C5	0.15352 (13)	0.11673 (14)	0.56030 (6)	0.0249 (3)	
H5	0.1458	0.0568	0.5298	0.030*	
C6	0.26998 (12)	0.14996 (12)	0.60080 (5)	0.0194 (2)	
C7	0.47004 (12)	0.16761 (12)	0.65481 (5)	0.0197 (2)	
C8	0.60830 (12)	0.13872 (13)	0.67854 (6)	0.0252 (3)	
H8A	0.6244	0.0564	0.7023	0.030*	
H8B	0.6391	0.1231	0.6469	0.030*	
C9	0.68619 (12)	0.35957 (13)	0.67806 (5)	0.0222 (3)	
H9A	0.6121	0.3650	0.6422	0.027*	
H9B	0.7624	0.3481	0.6684	0.027*	
C10	0.69630 (11)	0.48306 (13)	0.71274 (5)	0.0201 (2)	
C11	0.75372 (13)	0.68185 (14)	0.75169 (6)	0.0267 (3)	
C12	0.80865 (17)	0.80687 (16)	0.77019 (7)	0.0396 (4)	
H12	0.8685	0.8446	0.7562	0.047*	
C13	0.77203 (19)	0.87304 (16)	0.80967 (8)	0.0450 (4)	
H13	0.8071	0.9588	0.8232	0.054*	
C14	0.68394 (17)	0.81668 (16)	0.83043 (7)	0.0393 (4)	
H14	0.6612	0.8653	0.8578	0.047*	
C15	0.62941 (14)	0.69269 (15)	0.81217 (6)	0.0293 (3)	
H15	0.5702	0.6549	0.8265	0.035*	
C16	0.66544 (13)	0.62542 (13)	0.77169 (5)	0.0221 (3)	
C17	0.61070 (14)	0.63884 (13)	0.48431 (6)	0.0262 (3)	
C18	0.48772 (13)	0.67268 (13)	0.47497 (5)	0.0238 (3)	
H18	0.4208	0.6222	0.4489	0.029*	
C19	0.46257 (13)	0.78010 (13)	0.50371 (5)	0.0233 (3)	
C20	0.55850 (13)	0.86220 (13)	0.54417 (5)	0.0228 (3)	
C21	0.68386 (13)	0.81456 (14)	0.55233 (6)	0.0260 (3)	
C22	0.70968 (14)	0.71058 (15)	0.52261 (6)	0.0288 (3)	
H22	0.7941	0.6878	0.5281	0.035*	
C23	1.05744 (17)	0.6226 (2)	0.58074 (8)	0.0495 (5)	
H23A	1.0127	0.5755	0.5449	0.059*	
H23B	1.1415	0.5837	0.5987	0.059*	
H23C	1.0648	0.7183	0.5730	0.059*	
C24	0.98832 (15)	0.60810 (18)	0.61876 (7)	0.0371 (4)	
C25	1.0000	0.1051 (3)	0.7500	0.0971 (16)	
H25A	1.0691	0.0722	0.7836	0.116*	0.50
H25B	1.0110	0.0722	0.7154	0.116*	0.50
H25C	0.9199	0.0722	0.7511	0.116*	0.50

C26	1.0000	0.2497 (2)	0.7500	0.0355 (5)
H2N	0.4130 (16)	0.0525 (15)	0.5871 (7)	0.037 (5)*
H4N	0.8242 (14)	0.5947 (19)	0.6975 (7)	0.041 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.01758 (12)	0.01751 (13)	0.01522 (12)	0.000	0.00511 (9)	0.000
O1	0.0227 (5)	0.0215 (4)	0.0208 (4)	−0.0016 (3)	0.0046 (4)	−0.0025 (3)
O2	0.0533 (8)	0.0616 (9)	0.0637 (8)	0.0260 (7)	0.0257 (7)	−0.0152 (7)
O3	0.0612 (8)	0.0328 (6)	0.0310 (5)	0.0086 (5)	0.0194 (5)	−0.0069 (5)
O4	0.0274 (6)	0.0785 (10)	0.0554 (8)	−0.0016 (6)	0.0044 (6)	−0.0380 (7)
O5	0.0291 (6)	0.0489 (7)	0.0506 (7)	0.0037 (5)	0.0147 (5)	−0.0249 (6)
O6	0.0275 (5)	0.0275 (5)	0.0321 (5)	0.0021 (4)	0.0102 (4)	−0.0101 (4)
O7	0.0354 (6)	0.0790 (10)	0.0353 (6)	0.0055 (6)	0.0046 (5)	−0.0223 (6)
O8	0.0292 (6)	0.0469 (7)	0.0486 (7)	−0.0026 (5)	0.0126 (5)	0.0015 (5)
N1	0.0186 (5)	0.0204 (5)	0.0200 (5)	0.0016 (4)	0.0058 (4)	−0.0023 (4)
N2	0.0214 (5)	0.0189 (5)	0.0203 (5)	0.0001 (4)	0.0075 (4)	−0.0037 (4)
N3	0.0211 (5)	0.0207 (5)	0.0178 (5)	−0.0001 (4)	0.0082 (4)	−0.0005 (4)
N4	0.0287 (6)	0.0261 (6)	0.0286 (6)	−0.0045 (5)	0.0170 (5)	−0.0010 (5)
N5	0.0495 (8)	0.0292 (6)	0.0304 (6)	0.0138 (6)	0.0222 (6)	0.0023 (5)
N6	0.0251 (6)	0.0324 (6)	0.0345 (6)	0.0000 (5)	0.0100 (5)	−0.0109 (5)
N7	0.0271 (6)	0.0361 (7)	0.0327 (6)	0.0065 (5)	0.0061 (5)	−0.0024 (5)
N8	0.0477 (9)	0.0524 (9)	0.0459 (8)	0.0125 (7)	0.0295 (7)	0.0123 (7)
N9	0.0421 (12)	0.0387 (12)	0.0568 (13)	0.000	0.0132 (10)	0.000
C1	0.0192 (6)	0.0204 (6)	0.0178 (5)	−0.0006 (5)	0.0052 (5)	−0.0001 (4)
C2	0.0217 (6)	0.0300 (7)	0.0234 (6)	0.0023 (5)	0.0074 (5)	−0.0052 (5)
C3	0.0199 (6)	0.0351 (7)	0.0289 (7)	0.0021 (5)	0.0080 (5)	−0.0046 (6)
C4	0.0203 (6)	0.0330 (7)	0.0259 (6)	−0.0026 (5)	0.0035 (5)	−0.0040 (6)
C5	0.0247 (7)	0.0264 (6)	0.0215 (6)	−0.0022 (5)	0.0059 (5)	−0.0051 (5)
C6	0.0204 (6)	0.0191 (6)	0.0196 (5)	−0.0003 (4)	0.0082 (5)	0.0008 (4)
C7	0.0212 (6)	0.0167 (5)	0.0209 (6)	−0.0001 (5)	0.0073 (5)	−0.0009 (4)
C8	0.0206 (6)	0.0220 (6)	0.0294 (6)	0.0019 (5)	0.0049 (5)	−0.0078 (5)
C9	0.0217 (6)	0.0264 (7)	0.0198 (6)	0.0004 (5)	0.0091 (5)	−0.0015 (5)
C10	0.0189 (6)	0.0239 (6)	0.0179 (5)	0.0011 (5)	0.0073 (5)	0.0026 (5)
C11	0.0299 (7)	0.0246 (7)	0.0280 (6)	−0.0030 (5)	0.0133 (6)	−0.0004 (5)
C12	0.0469 (9)	0.0293 (8)	0.0490 (9)	−0.0132 (7)	0.0251 (8)	−0.0049 (7)
C13	0.0582 (11)	0.0270 (8)	0.0540 (10)	−0.0149 (7)	0.0254 (9)	−0.0139 (7)
C14	0.0509 (10)	0.0305 (8)	0.0415 (8)	−0.0047 (7)	0.0228 (8)	−0.0134 (7)
C15	0.0347 (8)	0.0284 (7)	0.0283 (6)	−0.0023 (6)	0.0156 (6)	−0.0056 (6)
C16	0.0240 (6)	0.0213 (6)	0.0211 (6)	−0.0010 (5)	0.0080 (5)	−0.0001 (5)
C17	0.0380 (8)	0.0225 (6)	0.0229 (6)	0.0085 (5)	0.0168 (6)	0.0030 (5)
C18	0.0335 (7)	0.0202 (6)	0.0203 (6)	0.0012 (5)	0.0130 (5)	0.0008 (5)
C19	0.0259 (7)	0.0229 (6)	0.0229 (6)	0.0037 (5)	0.0111 (5)	−0.0006 (5)
C20	0.0256 (7)	0.0230 (6)	0.0216 (6)	0.0032 (5)	0.0106 (5)	0.0002 (5)
C21	0.0252 (7)	0.0282 (7)	0.0238 (6)	0.0038 (5)	0.0081 (5)	0.0003 (5)
C22	0.0287 (7)	0.0332 (7)	0.0269 (6)	0.0109 (6)	0.0129 (6)	0.0036 (6)
C23	0.0350 (9)	0.0802 (14)	0.0412 (9)	0.0146 (9)	0.0233 (8)	0.0109 (9)

C24	0.0319 (8)	0.0471 (9)	0.0344 (8)	0.0142 (7)	0.0146 (7)	0.0100 (7)
C25	0.109 (3)	0.0309 (15)	0.110 (3)	0.000	−0.011 (3)	0.000
C26	0.0263 (10)	0.0338 (12)	0.0407 (11)	0.000	0.0052 (9)	0.000

Geometric parameters (Å, º)

Co—N1	2.0355 (10)	C4—H4	0.9500
Co—N1^{i}	2.0355 (10)	C5—C6	1.3910 (18)
Co—N3	2.0367 (11)	C5—H5	0.9500
Co—N3^{i}	2.0367 (11)	C7—C8	1.4993 (18)
O1—C8	1.4250 (15)	C8—H8A	0.9900
O1—C9	1.4272 (16)	C8—H8B	0.9900
O2—N5	1.2234 (19)	C9—C10	1.4849 (18)
O3—N5	1.2315 (18)	C9—H9A	0.9900
O4—N6	1.2278 (17)	C9—H9B	0.9900
O5—N6	1.2233 (16)	C11—C12	1.393 (2)
O6—C20	1.2475 (16)	C11—C16	1.3956 (19)
O7—N7	1.2255 (17)	C12—C13	1.375 (2)
O8—N7	1.2270 (17)	C12—H12	0.9500
N1—C7	1.3308 (16)	C13—C14	1.405 (3)
N1—C1	1.4048 (16)	C13—H13	0.9500
N2—C7	1.3416 (16)	C14—C15	1.381 (2)
N2—C6	1.3855 (16)	C14—H14	0.9500
N2—H2N	0.858 (9)	C15—C16	1.3977 (19)
N3—C10	1.3247 (15)	C15—H15	0.9500
N3—C16	1.4004 (16)	C17—C18	1.378 (2)
N4—C10	1.3404 (17)	C17—C22	1.388 (2)
N4—C11	1.3840 (18)	C18—C19	1.3756 (18)
N4—H4N	0.858 (9)	C18—H18	0.9500
N5—C17	1.4459 (17)	C19—C20	1.4469 (19)
N6—C19	1.4497 (18)	C20—C21	1.4492 (19)
N7—C21	1.4597 (19)	C21—C22	1.368 (2)
N8—C24	1.133 (2)	C22—H22	0.9500
N9—C26	1.121 (3)	C23—C24	1.450 (2)
C1—C2	1.3956 (18)	C23—H23A	0.9800
C1—C6	1.4013 (17)	C23—H23B	0.9800
C2—C3	1.3850 (19)	C23—H23C	0.9800
C2—H2	0.9500	C25—C26	1.436 (4)
C3—C4	1.405 (2)	C25—H25A	0.9800
C3—H3	0.9500	C25—H25B	0.9800
C4—C5	1.380 (2)	C25—H25C	0.9800
N1—Co—N1^{i}	113.22 (6)	C10—C9—H9A	110.5
N1—Co—N3	117.15 (4)	O1—C9—H9B	110.5
N1^{i}—Co—N3	106.14 (4)	C10—C9—H9B	110.5
N1—Co—N3^{i}	106.13 (4)	H9A—C9—H9B	108.7
N1^{i}—Co—N3^{i}	117.15 (4)	N3—C10—N4	112.81 (11)
N3—Co—N3^{i}	96.33 (6)	N3—C10—C9	122.03 (11)

C8—O1—C9	112.25 (10)	N4—C10—C9	125.15 (11)
C7—N1—C1	105.13 (10)	N4—C11—C12	131.85 (13)
C7—N1—Co	124.97 (9)	N4—C11—C16	105.85 (12)
C1—N1—Co	129.90 (8)	C12—C11—C16	122.27 (13)
C7—N2—C6	107.67 (10)	C13—C12—C11	116.71 (15)
C7—N2—H2N	124.2 (12)	C13—C12—H12	121.6
C6—N2—H2N	128.2 (12)	C11—C12—H12	121.6
C10—N3—C16	105.33 (10)	C12—C13—C14	121.49 (14)
C10—N3—Co	122.88 (9)	C12—C13—H13	119.3
C16—N3—Co	131.77 (8)	C14—C13—H13	119.3
C10—N4—C11	107.41 (11)	C15—C14—C13	121.90 (14)
C10—N4—H4N	126.7 (13)	C15—C14—H14	119.0
C11—N4—H4N	125.8 (13)	C13—C14—H14	119.0
O2—N5—O3	123.27 (13)	C14—C15—C16	116.89 (14)
O2—N5—C17	118.13 (14)	C14—C15—H15	121.6
O3—N5—C17	118.60 (13)	C16—C15—H15	121.6
O5—N6—O4	122.50 (13)	C11—C16—C15	120.73 (13)
O5—N6—C19	119.46 (12)	C11—C16—N3	108.58 (11)
O4—N6—C19	118.03 (12)	C15—C16—N3	130.67 (12)
O7—N7—O8	123.97 (14)	C18—C17—C22	121.11 (12)
O7—N7—C21	117.91 (13)	C18—C17—N5	119.33 (13)
O8—N7—C21	118.07 (12)	C22—C17—N5	119.56 (13)
C2—C1—C6	120.09 (12)	C19—C18—C17	119.49 (13)
C2—C1—N1	131.19 (11)	C19—C18—H18	120.3
C6—C1—N1	108.69 (11)	C17—C18—H18	120.3
C3—C2—C1	117.27 (12)	C18—C19—C20	123.90 (12)
C3—C2—H2	121.4	C18—C19—N6	115.93 (12)
C1—C2—H2	121.4	C20—C19—N6	120.12 (11)
C2—C3—C4	121.95 (13)	O6—C20—C19	125.89 (12)
C2—C3—H3	119.0	O6—C20—C21	122.06 (13)
C4—C3—H3	119.0	C19—C20—C21	111.92 (11)
C5—C4—C3	121.29 (12)	C22—C21—C20	124.43 (13)
C5—C4—H4	119.4	C22—C21—N7	116.92 (13)
C3—C4—H4	119.4	C20—C21—N7	118.64 (12)
C4—C5—C6	116.58 (12)	C21—C22—C17	119.00 (13)
C4—C5—H5	121.7	C21—C22—H22	120.5
C6—C5—H5	121.7	C17—C22—H22	120.5
N2—C6—C5	131.51 (12)	C24—C23—H23A	109.5
N2—C6—C1	105.68 (11)	C24—C23—H23B	109.5
C5—C6—C1	122.80 (12)	H23A—C23—H23B	109.5
N1—C7—N2	112.80 (11)	C24—C23—H23C	109.5
N1—C7—C8	124.00 (11)	H23A—C23—H23C	109.5
N2—C7—C8	123.12 (11)	H23B—C23—H23C	109.5
O1—C8—C7	109.64 (10)	N8—C24—C23	178.40 (18)
O1—C8—H8A	109.7	C26—C25—H25A	109.5
C7—C8—H8A	109.7	C26—C25—H25B	109.5
O1—C8—H8B	109.7	H25A—C25—H25B	109.5
C7—C8—H8B	109.7	C26—C25—H25C	109.5

H8A—C8—H8B	108.2	H25A—C25—H25C	109.5
O1—C9—C10	106.29 (10)	H25B—C25—H25C	109.5
O1—C9—H9A	110.5	N9—C26—C25	180.000 (3)
N1^{i}—Co—N1—C7	−63.92 (10)	O1—C9—C10—N4	141.87 (12)
N3—Co—N1—C7	60.12 (11)	C10—N4—C11—C12	178.52 (17)
N3^{i}—Co—N1—C7	166.22 (10)	C10—N4—C11—C16	0.22 (15)
N1^{i}—Co—N1—C1	116.01 (11)	N4—C11—C12—C13	−177.85 (17)
N3—Co—N1—C1	−119.95 (10)	C16—C11—C12—C13	0.2 (3)
N3^{i}—Co—N1—C1	−13.86 (11)	C11—C12—C13—C14	0.3 (3)
N1—Co—N3—C10	−29.43 (11)	C12—C13—C14—C15	−0.3 (3)
N1^{i}—Co—N3—C10	98.12 (10)	C13—C14—C15—C16	−0.3 (3)
N3^{i}—Co—N3—C10	−141.21 (11)	N4—C11—C16—C15	177.74 (13)
N1—Co—N3—C16	148.33 (10)	C12—C11—C16—C15	−0.8 (2)
N1^{i}—Co—N3—C16	−84.11 (11)	N4—C11—C16—N3	−0.97 (15)
N3^{i}—Co—N3—C16	36.55 (10)	C12—C11—C16—N3	−179.47 (14)
C7—N1—C1—C2	177.34 (14)	C14—C15—C16—C11	0.8 (2)
Co—N1—C1—C2	−2.6 (2)	C14—C15—C16—N3	179.14 (14)
C7—N1—C1—C6	−0.67 (13)	C10—N3—C16—C11	1.34 (14)
Co—N1—C1—C6	179.40 (8)	Co—N3—C16—C11	−176.71 (9)
C6—C1—C2—C3	0.0 (2)	C10—N3—C16—C15	−177.19 (14)
N1—C1—C2—C3	−177.80 (13)	Co—N3—C16—C15	4.8 (2)
C1—C2—C3—C4	−0.6 (2)	O2—N5—C17—C18	−172.99 (14)
C2—C3—C4—C5	0.3 (2)	O3—N5—C17—C18	6.38 (19)
C3—C4—C5—C6	0.6 (2)	O2—N5—C17—C22	7.5 (2)
C7—N2—C6—C5	−178.36 (14)	O3—N5—C17—C22	−173.11 (13)
C7—N2—C6—C1	0.86 (14)	C22—C17—C18—C19	0.6 (2)
C4—C5—C6—N2	177.88 (13)	N5—C17—C18—C19	−178.90 (12)
C4—C5—C6—C1	−1.2 (2)	C17—C18—C19—C20	−0.1 (2)
C2—C1—C6—N2	−178.38 (12)	C17—C18—C19—N6	177.32 (12)
N1—C1—C6—N2	−0.12 (13)	O5—N6—C19—C18	162.30 (14)
C2—C1—C6—C5	0.92 (19)	O4—N6—C19—C18	−19.0 (2)
N1—C1—C6—C5	179.19 (12)	O5—N6—C19—C20	−20.2 (2)
C1—N1—C7—N2	1.27 (14)	O4—N6—C19—C20	158.52 (15)
Co—N1—C7—N2	−178.79 (8)	C18—C19—C20—O6	173.77 (13)
C1—N1—C7—C8	−175.73 (12)	N6—C19—C20—O6	−3.5 (2)
Co—N1—C7—C8	4.21 (18)	C18—C19—C20—C21	−2.18 (18)
C6—N2—C7—N1	−1.38 (15)	N6—C19—C20—C21	−179.48 (12)
C6—N2—C7—C8	175.65 (12)	O6—C20—C21—C22	−171.77 (14)
C9—O1—C8—C7	−77.34 (13)	C19—C20—C21—C22	4.36 (19)
N1—C7—C8—O1	−26.34 (18)	O6—C20—C21—N7	7.1 (2)
N2—C7—C8—O1	156.97 (11)	C19—C20—C21—N7	−176.76 (12)
C8—O1—C9—C10	153.52 (10)	O7—N7—C21—C22	−140.26 (15)
C16—N3—C10—N4	−1.25 (14)	O8—N7—C21—C22	37.34 (19)
Co—N3—C10—N4	177.02 (8)	O7—N7—C21—C20	40.78 (19)
C16—N3—C10—C9	179.16 (11)	O8—N7—C21—C20	−141.62 (13)
Co—N3—C10—C9	−2.57 (16)	C20—C21—C22—C17	−4.2 (2)
C11—N4—C10—N3	0.67 (15)	N7—C21—C22—C17	176.93 (12)

C11—N4—C10—C9	−179.76 (12)	C18—C17—C22—C21	1.5 (2)
O1—C9—C10—N3	−38.59 (16)	N5—C17—C22—C21	−179.07 (12)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O6^{ii}	0.86 (1)	1.89 (1)	2.6746 (14)	151 (2)
N2—H2*N*···O5^{ii}	0.86 (1)	2.38 (2)	3.0166 (15)	131 (2)
N4—H4*N*···N8	0.86 (1)	2.05 (1)	2.9040 (18)	172 (2)

Symmetry code: (ii) *x*, *y*−1, *z*.