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Bis(methanol-κO)bis{5-(pyridin-2-yl-κN)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-1-ido-κN^1}-cobalt(II)

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Keywords: crystal structure; triazole; cobalt; hydrogen bonding.

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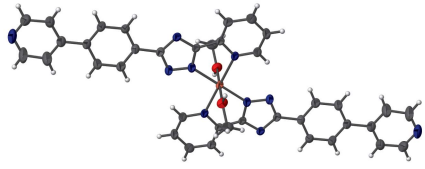
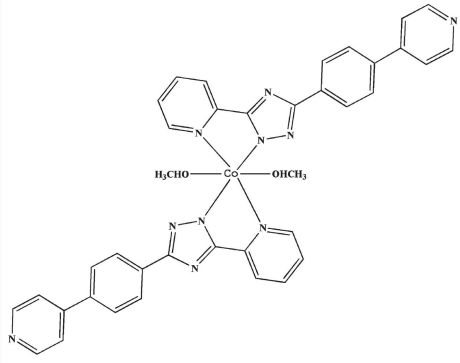
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title Co^{II} complex, $[Co(C_{18}H_{12}N_5)_2(CH_3OH)_2]$, contains one half-molecule, and the complex is completed by application of an inversion centre. The Co^{II} cation is coordinated by two deprotonated 1,2,4-triazole-based ligands, and two methanol molecules, in an N_4O_2 octahedral coordination geometry. Four N atoms are placed in the equatorial plane, while *trans*-methanol molecules occupy the axial positions. In the crystal, neighbouring complexes are linked *via* O—H···N hydrogen-bonding interactions, involving the methanol as donor and non-coordinating N triazole sites as acceptor groups, forming a two-dimensional network parallel to (100).

3D view



Chemical scheme



Structure description

The single-crystal X-ray diffraction analysis of the title complex reveals that the Co^{II} atom is six-coordinate. The metal is located on an inversion centre, forming a centrosymmetric complex with coordinating methanol molecules occupying *trans* sites (Fig. 1). The isotypic complex bearing water as ligands in place of methanol has been reported (Li, 2013*a*). However, for the water-containing complex, the triazole derivative was not planar, while this ligand is almost planar in the title complex. The same triazole derivative has also been used for the synthesis of Fe^{II} and Zn^{II} mononuclear complexes (Li, 2013*b*,*c*), and polymeric species (Zhang *et al.*, 2012, 2013). Multidentate ligands containing 1,2,4-trizaole heterocycle and other *N*-donor heterocyclic groups are frequently used in the preparation of metal complexes (Gong *et al.*, 2014; Liu *et al.*, 2015; Dong *et al.*, 2016).

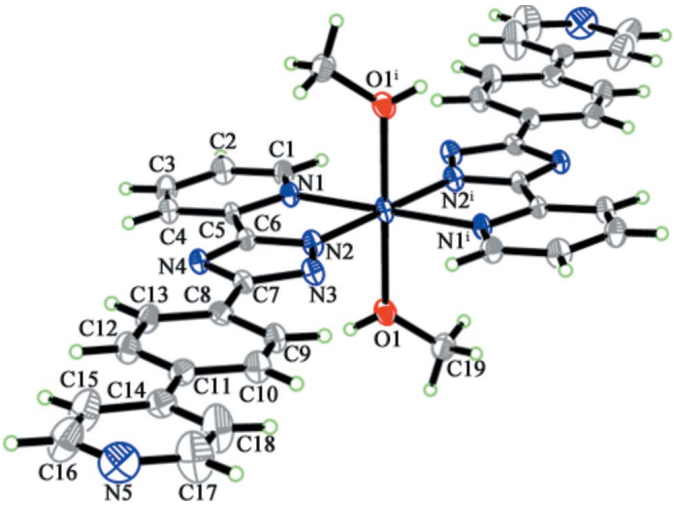


Figure 1
The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

The crystal structure features intermolecular O—H···N hydrogen bonds (Table 1) involving the hydroxyl group of MeOH and one triazole N atom, forming a two-dimensional network parallel to (100).

Synthesis and crystallization

A mixture of 5-(pyridin-2-yl)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazole (0.15 mmol, 0.0448 g), cobalt(II) nitrate hexahydrate (0.10 mmol, 0.0234 g) and CH_3OH (12 ml) were placed in a Teflon-lined stainless steel vessel, heated to 437 K for 3 d, followed by slow cooling to room temperature. Yellow prismatic crystals were obtained. Analysis calculated for $C_{38}H_{32}CoN_{10}O_2$: C 63.36, H 4.44, N 19.45%; found: C 63.52, H 4.48, N 19.45%

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4^{i}	0.85 (1)	1.92 (2)	2.760 (5)	168 (5)

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{18}H_{12}N_5)_2(CH_4O)_2]$
M_r	719.67
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	13.414 (4), 12.654 (3), 9.964 (1)
β (°)	101.43 (2)
V (Å^3)	1657.8 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.57
Crystal size (mm)	0.23 × 0.21 × 0.18
Data collection	
Diffractometer	Bruker *SMART* 1000 CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.880, 0.904
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17371, 3842, 2915
R_{int}	0.112
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.653
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.074, 0.193, 1.00
No. of reflections	3842
No. of parameters	235
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.55

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x161316 [doi:10.1107/S241431461601316X]

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Crystal data

$[Co(C_{18}H_{12}N_5)_2(CH_4O)_2]$
M_r = 719.67
Monoclinic, $P2_1/c$
a = 13.414 (4) Å
b = 12.654 (3) Å
c = 9.964 (1) Å
β = 101.43 (2)°
V = 1657.8 (7) Å^3
Z = 2
$F(000)$ = 746
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3457 reflections
θ = 2.2–27.5°
μ = 0.57 mm^{-1}
T = 296 K
Prism, yellow
0.23 × 0.21 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.880, T_{max} = 0.904
17371 measured reflections
3842 independent reflections
2915 reflections with $I > 2\sigma(I)$
R_{int} = 0.112
θ_{max} = 27.7°, θ_{min} = 2.6°
h = −17→17
k = −16→16
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.193
S = 1.00
3842 reflections
235 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0867P)^2 + 2.491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.0000	0.0276 (2)

O1	0.4016 (2)	0.5716 (2)	0.1228 (3)	0.0366 (6)
H1	0.398 (4)	0.6381 (10)	0.132 (5)	0.055*
N1	0.4240 (2)	0.3508 (2)	−0.0040 (3)	0.0279 (7)
N2	0.5827 (2)	0.4245 (2)	0.1702 (3)	0.0310 (7)
N3	0.6646 (2)	0.4464 (2)	0.2708 (3)	0.0315 (7)
N4	0.6079 (2)	0.2819 (2)	0.3071 (3)	0.0282 (7)
N5	1.1509 (3)	0.3720 (4)	1.0761 (4)	0.0662 (13)
C1	0.3465 (3)	0.3180 (3)	−0.1010 (4)	0.0334 (8)
H1A	0.3178	0.3651	−0.1694	0.040*
C2	0.3072 (3)	0.2164 (3)	−0.1036 (4)	0.0387 (9)
H2A	0.2534	0.1953	−0.1725	0.046*
C3	0.3500 (3)	0.1477 (3)	−0.0015 (4)	0.0399 (10)
H3B	0.3256	0.0789	−0.0018	0.048*
C4	0.4283 (3)	0.1795 (3)	0.1010 (4)	0.0337 (8)
H4B	0.4561	0.1336	0.1714	0.040*
C5	0.4649 (3)	0.2818 (3)	0.0968 (4)	0.0255 (7)
C6	0.5516 (3)	0.3269 (3)	0.1939 (3)	0.0264 (7)
C7	0.6775 (3)	0.3599 (3)	0.3507 (4)	0.0277 (7)
C8	0.7604 (3)	0.3551 (3)	0.4717 (4)	0.0299 (8)
C9	0.8303 (3)	0.4378 (3)	0.4960 (4)	0.0364 (9)
H9A	0.8252	0.4930	0.4335	0.044*
C10	0.9068 (3)	0.4394 (3)	0.6113 (4)	0.0412 (10)
H10A	0.9520	0.4958	0.6250	0.049*
C11	0.9178 (3)	0.3579 (3)	0.7077 (4)	0.0353 (9)
C12	0.8490 (3)	0.2738 (4)	0.6814 (4)	0.0412 (10)
H12A	0.8553	0.2175	0.7426	0.049*
C13	0.7711 (3)	0.2723 (3)	0.5654 (4)	0.0358 (9)
H13A	0.7261	0.2156	0.5507	0.043*
C14	0.9990 (3)	0.3617 (4)	0.8330 (4)	0.0404 (10)
C15	1.0129 (4)	0.2820 (5)	0.9295 (5)	0.0670 (17)
H15A	0.9722	0.2220	0.9157	0.080*
C16	1.0886 (4)	0.2912 (6)	1.0489 (6)	0.076 (2)
H16A	1.0949	0.2367	1.1125	0.091*
C17	1.1400 (5)	0.4469 (5)	0.9823 (6)	0.080 (2)
H17A	1.1837	0.5046	0.9979	0.096*
C18	1.0668 (5)	0.4453 (5)	0.8609 (6)	0.0734 (18)
H18A	1.0636	0.5005	0.7986	0.088*
C19	0.3625 (4)	0.5204 (3)	0.2296 (5)	0.0445 (10)
H19A	0.3210	0.5691	0.2682	0.067*
H19B	0.4180	0.4971	0.2996	0.067*
H19C	0.3222	0.4605	0.1927	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0360 (4)	0.0185 (3)	0.0245 (4)	−0.0016 (3)	−0.0034 (3)	0.0023 (3)
O1	0.0509 (17)	0.0258 (14)	0.0336 (14)	0.0025 (12)	0.0100 (13)	−0.0025 (11)
N1	0.0338 (16)	0.0222 (15)	0.0246 (15)	−0.0017 (12)	−0.0020 (13)	0.0029 (11)

N2	0.0351 (17)	0.0245 (15)	0.0294 (16)	−0.0022 (12)	−0.0036 (14)	0.0007 (12)
N3	0.0360 (17)	0.0251 (16)	0.0290 (16)	−0.0004 (13)	−0.0043 (14)	−0.0003 (12)
N4	0.0335 (16)	0.0230 (15)	0.0265 (15)	0.0001 (12)	0.0021 (13)	0.0039 (11)
N5	0.052 (3)	0.092 (4)	0.044 (2)	−0.005 (2)	−0.015 (2)	0.002 (2)
C1	0.034 (2)	0.031 (2)	0.0311 (19)	−0.0014 (15)	−0.0019 (16)	0.0038 (15)
C2	0.039 (2)	0.037 (2)	0.034 (2)	−0.0082 (17)	−0.0060 (18)	−0.0045 (17)
C3	0.048 (2)	0.028 (2)	0.042 (2)	−0.0094 (17)	0.005 (2)	−0.0016 (16)
C4	0.041 (2)	0.0261 (19)	0.0324 (19)	−0.0020 (15)	0.0035 (17)	0.0044 (15)
C5	0.0308 (18)	0.0193 (16)	0.0257 (17)	0.0013 (13)	0.0041 (14)	0.0037 (13)
C6	0.0312 (18)	0.0228 (17)	0.0239 (17)	0.0016 (14)	0.0027 (14)	0.0030 (13)
C7	0.0321 (19)	0.0249 (17)	0.0250 (17)	0.0039 (14)	0.0031 (15)	−0.0001 (13)
C8	0.0286 (18)	0.0310 (19)	0.0281 (18)	0.0020 (14)	0.0010 (15)	−0.0012 (14)
C9	0.041 (2)	0.030 (2)	0.035 (2)	−0.0015 (16)	−0.0002 (17)	0.0049 (15)
C10	0.041 (2)	0.039 (2)	0.038 (2)	−0.0078 (18)	−0.0053 (19)	0.0011 (17)
C11	0.0308 (19)	0.045 (2)	0.0284 (19)	−0.0004 (16)	0.0015 (16)	0.0031 (16)
C12	0.042 (2)	0.046 (2)	0.031 (2)	−0.0021 (18)	−0.0049 (18)	0.0109 (18)
C13	0.037 (2)	0.039 (2)	0.0290 (19)	−0.0073 (16)	0.0007 (17)	0.0056 (16)
C14	0.036 (2)	0.049 (2)	0.034 (2)	0.0000 (18)	0.0024 (18)	0.0002 (18)
C15	0.055 (3)	0.084 (4)	0.051 (3)	−0.028 (3)	−0.015 (3)	0.023 (3)
C16	0.055 (3)	0.111 (5)	0.053 (3)	−0.022 (3)	−0.012 (3)	0.037 (3)
C17	0.083 (4)	0.073 (4)	0.062 (4)	−0.020 (3)	−0.036 (3)	0.007 (3)
C18	0.076 (4)	0.061 (4)	0.066 (4)	−0.023 (3)	−0.028 (3)	0.014 (3)
C19	0.054 (3)	0.038 (2)	0.045 (2)	−0.0061 (19)	0.017 (2)	−0.0009 (18)

Geometric parameters (Å, º)

Co1—N2	2.067 (3)	C5—C6	1.473 (5)
Co1—N2^{i}	2.067 (3)	C7—C8	1.471 (5)
Co1—N1^{i}	2.142 (3)	C8—C13	1.392 (5)
Co1—N1	2.142 (3)	C8—C9	1.394 (5)
Co1—O1^{i}	2.168 (3)	C9—C10	1.381 (6)
Co1—O1	2.168 (3)	C9—H9A	0.9300
O1—C19	1.432 (5)	C10—C11	1.396 (6)
O1—H1	0.849 (10)	C10—H10A	0.9300
N1—C1	1.338 (5)	C11—C12	1.400 (6)
N1—C5	1.362 (4)	C11—C14	1.486 (6)
N2—C6	1.339 (5)	C12—C13	1.396 (5)
N2—N3	1.361 (4)	C12—H12A	0.9300
N3—C7	1.344 (5)	C13—H13A	0.9300
N4—C6	1.353 (4)	C14—C15	1.380 (7)
N4—C7	1.369 (5)	C14—C18	1.387 (7)
N5—C16	1.314 (8)	C15—C16	1.407 (7)
N5—C17	1.320 (8)	C15—H15A	0.9300
C1—C2	1.388 (6)	C16—H16A	0.9300
C1—H1A	0.9300	C17—C18	1.399 (7)
C2—C3	1.374 (6)	C17—H17A	0.9300
C2—H2A	0.9300	C18—H18A	0.9300
C3—C4	1.372 (6)	C19—H19A	0.9600

C3—H3B	0.9300	C19—H19B	0.9600
C4—C5	1.388 (5)	C19—H19C	0.9600
C4—H4B	0.9300		

N2—Co1—N2^{i}	180.0	N4—C6—C5	128.5 (3)
N2—Co1—N1^{i}	102.48 (12)	N3—C7—N4	113.6 (3)
N2^{i}—Co1—N1^{i}	77.52 (12)	N3—C7—C8	120.5 (3)
N2—Co1—N1	77.52 (12)	N4—C7—C8	125.9 (3)
N2^{i}—Co1—N1	102.48 (12)	C13—C8—C9	118.2 (4)
N1^{i}—Co1—N1	180.00 (16)	C13—C8—C7	122.8 (3)
N2—Co1—O1^{i}	88.97 (14)	C9—C8—C7	119.0 (3)
N2^{i}—Co1—O1^{i}	91.03 (14)	C10—C9—C8	121.3 (4)
N1^{i}—Co1—O1^{i}	92.20 (13)	C10—C9—H9A	119.4
N1—Co1—O1^{i}	87.80 (13)	C8—C9—H9A	119.4
N2—Co1—O1	91.03 (14)	C9—C10—C11	121.4 (4)
N2^{i}—Co1—O1	88.97 (14)	C9—C10—H10A	119.3
N1^{i}—Co1—O1	87.80 (13)	C11—C10—H10A	119.3
N1—Co1—O1	92.20 (13)	C10—C11—C12	117.2 (4)
O1^{i}—Co1—O1	180.00 (11)	C10—C11—C14	121.0 (4)
C19—O1—Co1	125.7 (3)	C12—C11—C14	121.8 (4)
C19—O1—H1	109 (3)	C13—C12—C11	121.5 (4)
Co1—O1—H1	122 (3)	C13—C12—H12A	119.2
C1—N1—C5	118.4 (3)	C11—C12—H12A	119.2
C1—N1—Co1	125.9 (2)	C12—C13—C8	120.4 (4)
C5—N1—Co1	115.5 (2)	C12—C13—H13A	119.8
C6—N2—N3	107.0 (3)	C8—C13—H13A	119.8
C6—N2—Co1	115.8 (2)	C15—C14—C18	115.1 (4)
N3—N2—Co1	137.2 (2)	C15—C14—C11	122.6 (4)
C7—N3—N2	105.1 (3)	C18—C14—C11	122.3 (4)
C6—N4—C7	101.2 (3)	C14—C15—C16	120.3 (5)
C16—N5—C17	115.8 (5)	C14—C15—H15A	119.8
N1—C1—C2	122.6 (3)	C16—C15—H15A	119.8
N1—C1—H1A	118.7	N5—C16—C15	124.2 (5)
C2—C1—H1A	118.7	N5—C16—H16A	117.9
C3—C2—C1	118.0 (4)	C15—C16—H16A	117.9
C3—C2—H2A	121.0	N5—C17—C18	124.2 (6)
C1—C2—H2A	121.0	N5—C17—H17A	117.9
C4—C3—C2	120.8 (4)	C18—C17—H17A	117.9
C4—C3—H3B	119.6	C14—C18—C17	120.3 (5)
C2—C3—H3B	119.6	C14—C18—H18A	119.8
C3—C4—C5	118.3 (4)	C17—C18—H18A	119.8
C3—C4—H4B	120.8	O1—C19—H19A	109.5
C5—C4—H4B	120.8	O1—C19—H19B	109.5
N1—C5—C4	121.8 (3)	H19A—C19—H19B	109.5
N1—C5—C6	112.7 (3)	O1—C19—H19C	109.5
C4—C5—C6	125.5 (3)	H19A—C19—H19C	109.5
N2—C6—N4	113.2 (3)	H19B—C19—H19C	109.5
N2—C6—C5	118.3 (3)		

N2—Co1—O1—C19	−40.9 (3)	C7—N4—C6—N2	−0.7 (4)
N2^{i}—Co1—O1—C19	139.1 (3)	C7—N4—C6—C5	178.2 (4)
N1^{i}—Co1—O1—C19	−143.3 (3)	N1—C5—C6—N2	−3.0 (5)
N1—Co1—O1—C19	36.7 (3)	C4—C5—C6—N2	175.0 (4)
N2—Co1—N1—C1	−176.5 (3)	N1—C5—C6—N4	178.2 (4)
N2^{i}—Co1—N1—C1	3.5 (3)	C4—C5—C6—N4	−3.8 (6)
O1^{i}—Co1—N1—C1	−87.1 (3)	N2—N3—C7—N4	0.2 (4)
O1—Co1—N1—C1	92.9 (3)	N2—N3—C7—C8	180.0 (3)
N2—Co1—N1—C5	−1.8 (3)	C6—N4—C7—N3	0.3 (4)
N2^{i}—Co1—N1—C5	178.2 (3)	C6—N4—C7—C8	−179.5 (4)
O1^{i}—Co1—N1—C5	87.7 (3)	N3—C7—C8—C13	173.3 (4)
O1—Co1—N1—C5	−92.3 (3)	N4—C7—C8—C13	−6.9 (6)
N1^{i}—Co1—N2—C6	−179.9 (3)	N3—C7—C8—C9	−5.1 (6)
N1—Co1—N2—C6	0.1 (3)	N4—C7—C8—C9	174.7 (4)
O1^{i}—Co1—N2—C6	−87.9 (3)	C13—C8—C9—C10	−1.4 (6)
O1—Co1—N2—C6	92.1 (3)	C7—C8—C9—C10	177.1 (4)
N1^{i}—Co1—N2—N3	−0.3 (4)	C8—C9—C10—C11	0.4 (7)
N1—Co1—N2—N3	179.7 (4)	C9—C10—C11—C12	1.1 (7)
O1^{i}—Co1—N2—N3	91.7 (4)	C9—C10—C11—C14	−178.5 (4)
O1—Co1—N2—N3	−88.3 (4)	C10—C11—C12—C13	−1.5 (7)
C6—N2—N3—C7	−0.6 (4)	C14—C11—C12—C13	178.1 (4)
Co1—N2—N3—C7	179.8 (3)	C11—C12—C13—C8	0.5 (7)
C5—N1—C1—C2	−0.8 (6)	C9—C8—C13—C12	0.9 (6)
Co1—N1—C1—C2	173.8 (3)	C7—C8—C13—C12	−177.4 (4)
N1—C1—C2—C3	0.3 (7)	C10—C11—C14—C15	−179.1 (5)
C1—C2—C3—C4	0.9 (7)	C12—C11—C14—C15	1.3 (7)
C2—C3—C4—C5	−1.7 (6)	C10—C11—C14—C18	0.4 (7)
C1—N1—C5—C4	0.0 (5)	C12—C11—C14—C18	−179.2 (5)
Co1—N1—C5—C4	−175.2 (3)	C18—C14—C15—C16	2.8 (9)
C1—N1—C5—C6	178.1 (3)	C11—C14—C15—C16	−177.7 (5)
Co1—N1—C5—C6	3.0 (4)	C17—N5—C16—C15	−0.7 (10)
C3—C4—C5—N1	1.3 (6)	C14—C15—C16—N5	−1.3 (11)
C3—C4—C5—C6	−176.6 (4)	C16—N5—C17—C18	1.1 (11)
N3—N2—C6—N4	0.8 (4)	C15—C14—C18—C17	−2.5 (9)
Co1—N2—C6—N4	−179.5 (2)	C11—C14—C18—C17	178.0 (6)
N3—N2—C6—C5	−178.2 (3)	N5—C17—C18—C14	0.6 (12)
Co1—N2—C6—C5	1.5 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N4^{ii}	0.85 (1)	1.92 (2)	2.760 (5)	168 (5)

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