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Diazidobis(2,2′-bipyridine)cobalt(III) perchlorate

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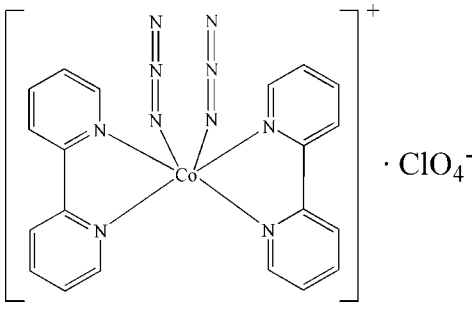
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.142; data-to-parameter ratio = 12.9.

In the title monomeric compound, $[Co(N_3)_2(C_{10}H_8N_2)_2]ClO_4$, the Co^{III} ion has a distorted octahedral coordination geometry formed by four N atoms from two chelating bipyridine ligands and two N atoms from azide groups, with the two azide groups in *cis* positions. The crystal structure is stabilized by weak C—H···O and C—H···N hydrogen bonding.

Related literature

For general background, see: Aebersold *et al.* (1998); Baffert *et al.* (2001); Zhang *et al.* (2000). For related structures, see: Chen (2002); Cheng *et al.* (2004); Jian *et al.* (2004, 2005); Tang *et al.* (2004); Urtiaga *et al.* (1995).



Experimental

Crystal data

$[Co(N_3)_2(C_{10}H_8N_2)_2]ClO_4$
M_r = 554.81
Monoclinic, $P2_1/n$
a = 15.0375 (17) Å
b = 8.1402 (9) Å
c = 18.966 (2) Å
β = 101.970 (1)°
V = 2271.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 291 (2) K
0.31 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.761, T_{max} = 0.894
14394 measured reflections
4180 independent reflections
3043 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.142
S = 1.03
4180 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	1.935 (3)	Co1—N5	1.947 (3)
Co1—N4	1.941 (3)	Co1—N3	1.948 (3)
Co1—N8	1.942 (3)	Co1—N2	1.949 (3)
N1—Co1—N4	178.80 (11)	N8—Co1—N3	87.51 (12)
N1—Co1—N8	91.71 (12)	N5—Co1—N3	174.91 (12)
N4—Co1—N8	88.34 (12)	N1—Co1—N2	82.47 (12)
N1—Co1—N5	88.79 (12)	N4—Co1—N2	97.44 (12)
N4—Co1—N5	92.41 (12)	N8—Co1—N2	173.90 (12)
N8—Co1—N5	92.31 (13)	N5—Co1—N2	89.40 (12)
N1—Co1—N3	96.30 (12)	N3—Co1—N2	91.30 (12)
N4—Co1—N3	82.50 (12)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N8	0.93	2.38	2.906 (5)	115
C11—H11···N10^{i}	0.93	2.36	3.142 (6)	141
C13—H13···O2^{ii}	0.93	2.56	3.322 (6)	139
C14—H14···O1^{iii}	0.93	2.46	3.305 (6)	152
C17—H17···O1^{iii}	0.93	2.55	3.430 (6)	157
C18—H18···O1^{iv}	0.93	2.47	3.326 (6)	154
C20—H20···N5	0.93	2.43	2.938 (5)	114

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: XU2329).

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supplementary materials

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Diazidobis(2,2'-bipyridine)cobalt(III) perchlorate

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Comment

At present, studies on self-assembly processes involving metal ions and inorganic or organic ligands have intensely attracted much attention in the fields of supramolecular chemistry and crystal engineering. The azide anion as an excellent versatile inorganic ligand has synthesized a great deal of compounds with attractive structural diversity, which possess potential application on metalloenzymes, and antiferromagnetic or ferromagnetic type interactions between the metallic centres (Baffert *et al.*, 2001; Zhang *et al.*, 2000; Aebersold *et al.*, 1998). Many complexes with the pseudohalide azide anion N_3^- and 2,2'-bipyridine ligand have been synthesized and their structure have been reported, such as $[Cd(N_3)_2(C_{10}H_8N_2)_2]$ (Jian *et al.*, 2005), $[Mn(N_3)_2(C_{10}H_8N_2)_2]$ (Cheng *et al.*, 2004), $[Zn(N_3)_2(C_{10}H_8N_2)_2]\cdot H_2O$ (Jian *et al.*, 2004) and $[Ni(N_3)_2(C_{10}H_8N_2)_2]\cdot H_2O$ (Urtiaga *et al.*, 1995). In this paper, we report the crystal structure of the title compound.

The asymmetric unit of crystal of the title compound comprises one mononuclear cobalt complex and one perchlorate (Fig. 1). The Co^{III} cation is six-coordinated to four N atoms from two chelating 2,2'-bipyridyl ligands and two other N atoms from two azide anion ligands. The two 2,2'-bipyridine ligands are bonded in bidentate mode to cobalt, forming five-membered chelate rings. Selected geometric parameters are listed in Table 1. The distances of four dative Co—N are not much different from that of the two Co—N_{azide}. The metal ion and six N atoms form a distorted octahedral geometry with the Co—N bond lengths in the range from 1.935 (3) to 1.949 (3) Å. The two azide ligands are practically linear [N7—N6···N5 (177.0 (4) °), N10—N9···N8 (176.2 (4) °)], which occupy *cis*-positions in the coordination polyhedron. No hydrogen bonding occurs between the Co complex cation and perchlorate anion. The similar coordination mode are observed in the structures of $[Co(N_3)_2(C_{10}H_8N_2)_2]\cdot Cl\cdot 2H_2O$ (Tang *et al.*, 2004), $[Co(N_3)_2(C_{10}H_8N_2)_2]\cdot NO_3\cdot 2H_2O$ (Chen, 2002).

In this crystal structure, there are some weak C—H···O and C—H···N hydrogen-bond interactions (Table 2), all of which stabilize the crystal structure.

Experimental

The complex was synthesized hydrothermally under autogenous pressure. A mixture of cobalt(II) perchlorate hexahydrate (73.2 mg, 0.2 mmol), 2,2'-bipyridine (62.4 mg, 0.4 mmol), sodium azide (26.4 mg, 0.4 mmol), 3,5-pyrazoledicarboxylic acid (34.8 mg, 0.2 mmol) and H_2O (15 ml) was sealed in a 40 ml stainless steel reactor with a Teflon liner and heated directly to 433 K. After maintaining this temperature for 72 h, the mixture was cooled slowly to room temperature at a rate of 5 $K.h^{-}$. Pink block-shaped crystals were obtained by filtration in 40% yield. Analysis calculated for $C_{20}H_{16}ClCoN_{10}O_4$(%): C 43.30, H 2.91, N 25.25; found: C 43.24, H 2.89, N 25.21.

Refinement

All H atoms were placed in geometrically idealized positions with C—H = 0.93 Å and refined in the riding-model approximation, $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

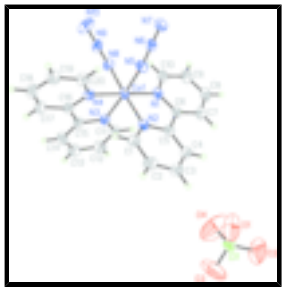


Fig. 1. The structure of complex (I), with displacement ellipsoids drawn at the 30% probability level.

Diazidobis(2,2'-bipyridine)cobalt(III) perchlorate

Crystal data

$[Co(N_3)_2(C_{10}H_8N_2)_2]ClO_4$	F_{000} = 1128
M_r = 554.81	D_x = 1.623 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2749 reflections
a = 15.0375 (17) Å	θ = 2.7–21.4°
b = 8.1402 (9) Å	μ = 0.93 mm^{-1}
c = 18.966 (2) Å	T = 291 (2) K
β = 101.970 (1)°	Block, pink
V = 2271.1 (4) Å^3	0.31 × 0.21 × 0.12 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4180 independent reflections
Radiation source: fine-focus sealed tube	3043 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 291(2) K	θ_{max} = 25.5°
φ and ω scans	θ_{min} = 2.7°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→18
T_{min} = 0.761, T_{max} = 0.894	k = −9→9
14394 measured reflections	l = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.142	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 1.0728P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4180 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl1	0.57781 (7)	0.81455 (13)	0.15942 (5)	0.0604 (3)
O1	0.6113 (4)	0.6733 (5)	0.1936 (3)	0.159 (2)
O2	0.5838 (5)	0.9370 (6)	0.2087 (3)	0.195 (3)
O3	0.6181 (6)	0.8543 (12)	0.1072 (4)	0.263 (5)
O4	0.4896 (4)	0.7874 (8)	0.1272 (5)	0.229 (4)
Co1	0.20342 (3)	−0.00720 (5)	0.04533 (2)	0.03801 (18)
N1	0.15295 (19)	0.1446 (4)	0.10508 (14)	0.0418 (7)
N2	0.30938 (19)	0.1351 (3)	0.07175 (14)	0.0417 (7)
N3	0.16283 (18)	0.1110 (3)	−0.04490 (15)	0.0412 (7)
N4	0.25327 (18)	−0.1564 (3)	−0.01633 (15)	0.0408 (7)
N5	0.2487 (2)	−0.1398 (4)	0.13068 (16)	0.0495 (8)
N6	0.1938 (2)	−0.1810 (4)	0.16520 (16)	0.0500 (8)
N7	0.1441 (3)	−0.2227 (5)	0.20088 (19)	0.0715 (10)
N8	0.0904 (2)	−0.1302 (4)	0.02225 (16)	0.0465 (7)
N9	0.09487 (19)	−0.2771 (4)	0.02498 (16)	0.0488 (8)
N10	0.0945 (3)	−0.4182 (5)	0.0286 (3)	0.0877 (13)
C1	0.3899 (3)	0.1159 (5)	0.0523 (2)	0.0542 (10)
H1	0.3980	0.0271	0.0235	0.065*
C2	0.4604 (3)	0.2238 (6)	0.0740 (2)	0.0632 (11)
H2	0.5154	0.2074	0.0599	0.076*
C3	0.4496 (3)	0.3554 (6)	0.1163 (2)	0.0641 (11)
H3	0.4967	0.4301	0.1306	0.077*
C4	0.3675 (3)	0.3757 (5)	0.1373 (2)	0.0573 (10)
H4	0.3588	0.4637	0.1664	0.069*
C5	0.2985 (2)	0.2634 (4)	0.11455 (17)	0.0438 (8)
C6	0.2093 (2)	0.2669 (4)	0.13491 (17)	0.0429 (8)

C7	0.1844 (3)	0.3782 (5)	0.1817 (2)	0.0536 (10)
H7	0.2236	0.4627	0.2010	0.064*
C8	0.1004 (3)	0.3628 (5)	0.1999 (2)	0.0614 (11)
H8	0.0828	0.4357	0.2322	0.074*
C9	0.0433 (3)	0.2389 (6)	0.1697 (2)	0.0612 (11)
H9	−0.0136	0.2272	0.1811	0.073*
C10	0.0711 (3)	0.1316 (5)	0.1222 (2)	0.0525 (9)
H10	0.0320	0.0482	0.1015	0.063*
C11	0.1199 (3)	0.2562 (5)	−0.0540 (2)	0.0526 (9)
H11	0.1102	0.3125	−0.0135	0.063*
C12	0.0897 (3)	0.3244 (5)	−0.1206 (2)	0.0624 (11)
H12	0.0602	0.4254	−0.1251	0.075*
C13	0.1034 (3)	0.2427 (6)	−0.1806 (2)	0.0728 (13)
H13	0.0834	0.2873	−0.2263	0.087*
C14	0.1472 (3)	0.0933 (6)	−0.1720 (2)	0.0632 (11)
H14	0.1564	0.0352	−0.2122	0.076*
C15	0.1775 (2)	0.0299 (4)	−0.10371 (19)	0.0450 (8)
C16	0.2262 (2)	−0.1256 (4)	−0.08716 (18)	0.0422 (8)
C17	0.2435 (3)	−0.2360 (5)	−0.1382 (2)	0.0581 (10)
H17	0.2243	−0.2139	−0.1871	0.070*
C18	0.2896 (3)	−0.3788 (5)	−0.1157 (2)	0.0642 (11)
H18	0.3002	−0.4558	−0.1492	0.077*
C19	0.3195 (3)	−0.4068 (5)	−0.0437 (2)	0.0599 (11)
H19	0.3525	−0.5010	−0.0277	0.072*
C20	0.3001 (2)	−0.2938 (5)	0.0048 (2)	0.0508 (9)
H20	0.3201	−0.3134	0.0538	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0696 (7)	0.0567 (6)	0.0549 (6)	0.0027 (5)	0.0127 (5)	0.0042 (5)
O1	0.255 (6)	0.086 (3)	0.104 (3)	0.066 (3)	−0.038 (3)	−0.006 (3)
O2	0.348 (9)	0.079 (3)	0.156 (5)	0.010 (5)	0.048 (5)	−0.049 (4)
O3	0.288 (9)	0.394 (12)	0.145 (5)	−0.100 (9)	0.130 (6)	0.037 (7)
O4	0.100 (4)	0.178 (6)	0.353 (11)	−0.004 (4)	−0.083 (5)	0.016 (6)
Co1	0.0382 (3)	0.0406 (3)	0.0342 (3)	0.0025 (2)	0.00499 (19)	−0.00220 (19)
N1	0.0430 (16)	0.0463 (17)	0.0351 (15)	0.0052 (13)	0.0059 (12)	−0.0004 (13)
N2	0.0433 (16)	0.0449 (17)	0.0359 (15)	0.0002 (13)	0.0060 (12)	0.0006 (13)
N3	0.0425 (16)	0.0400 (16)	0.0387 (15)	0.0044 (13)	0.0031 (12)	−0.0021 (13)
N4	0.0420 (16)	0.0398 (16)	0.0400 (15)	0.0029 (13)	0.0072 (12)	0.0006 (13)
N5	0.0480 (18)	0.057 (2)	0.0420 (16)	0.0055 (15)	0.0065 (14)	0.0082 (15)
N6	0.059 (2)	0.0506 (19)	0.0377 (16)	−0.0017 (16)	0.0036 (15)	−0.0022 (14)
N7	0.085 (3)	0.081 (3)	0.050 (2)	−0.019 (2)	0.0189 (19)	0.0043 (19)
N8	0.0432 (17)	0.0416 (19)	0.0523 (18)	0.0008 (14)	0.0047 (13)	−0.0041 (14)
N9	0.0409 (17)	0.054 (2)	0.0514 (18)	−0.0035 (15)	0.0089 (14)	−0.0128 (16)
N10	0.077 (3)	0.049 (2)	0.134 (4)	−0.005 (2)	0.014 (3)	−0.021 (3)
C1	0.050 (2)	0.057 (2)	0.057 (2)	−0.0012 (19)	0.0148 (18)	−0.0039 (19)
C2	0.045 (2)	0.073 (3)	0.073 (3)	−0.008 (2)	0.014 (2)	−0.002 (2)

C3	0.061 (3)	0.069 (3)	0.061 (3)	−0.023 (2)	0.008 (2)	0.002 (2)
C4	0.066 (3)	0.052 (2)	0.052 (2)	−0.011 (2)	0.0073 (19)	−0.0047 (18)
C5	0.049 (2)	0.044 (2)	0.0361 (18)	−0.0011 (16)	0.0041 (15)	0.0023 (16)
C6	0.050 (2)	0.044 (2)	0.0327 (17)	0.0062 (16)	0.0034 (15)	0.0012 (15)
C7	0.062 (2)	0.050 (2)	0.046 (2)	0.0061 (19)	0.0028 (18)	−0.0080 (18)
C8	0.070 (3)	0.062 (3)	0.052 (2)	0.018 (2)	0.013 (2)	−0.010 (2)
C9	0.054 (2)	0.074 (3)	0.058 (2)	0.012 (2)	0.0173 (19)	−0.010 (2)
C10	0.048 (2)	0.060 (3)	0.050 (2)	0.0028 (18)	0.0107 (17)	−0.0054 (18)
C11	0.061 (2)	0.042 (2)	0.053 (2)	0.0079 (18)	0.0083 (18)	−0.0021 (17)
C12	0.073 (3)	0.048 (2)	0.061 (3)	0.012 (2)	0.003 (2)	0.013 (2)
C13	0.094 (3)	0.068 (3)	0.051 (2)	0.007 (3)	0.004 (2)	0.017 (2)
C14	0.086 (3)	0.061 (3)	0.042 (2)	0.011 (2)	0.013 (2)	0.005 (2)
C15	0.050 (2)	0.044 (2)	0.0405 (19)	0.0015 (16)	0.0085 (16)	0.0018 (16)
C16	0.0434 (19)	0.043 (2)	0.0416 (19)	0.0020 (16)	0.0130 (15)	−0.0022 (16)
C17	0.067 (3)	0.063 (3)	0.045 (2)	0.009 (2)	0.0123 (19)	−0.0076 (19)
C18	0.071 (3)	0.058 (3)	0.067 (3)	0.007 (2)	0.023 (2)	−0.017 (2)
C19	0.060 (2)	0.052 (3)	0.071 (3)	0.016 (2)	0.021 (2)	0.001 (2)
C20	0.051 (2)	0.048 (2)	0.053 (2)	0.0103 (18)	0.0096 (17)	0.0009 (18)

Geometric parameters (Å, °)

Cl1—O3	1.304 (5)	C4—C5	1.383 (5)
Cl1—O2	1.357 (5)	C4—H4	0.9300
Cl1—O4	1.359 (5)	C5—C6	1.472 (5)
Cl1—O1	1.364 (4)	C6—C7	1.373 (5)
Co1—N1	1.935 (3)	C7—C8	1.383 (6)
Co1—N4	1.941 (3)	C7—H7	0.9300
Co1—N8	1.942 (3)	C8—C9	1.371 (6)
Co1—N5	1.947 (3)	C8—H8	0.9300
Co1—N3	1.948 (3)	C9—C10	1.380 (5)
Co1—N2	1.949 (3)	C9—H9	0.9300
N1—C10	1.341 (4)	C10—H10	0.9300
N1—C6	1.353 (4)	C11—C12	1.369 (5)
N2—C1	1.346 (4)	C11—H11	0.9300
N2—C5	1.353 (4)	C12—C13	1.370 (6)
N3—C11	1.341 (4)	C12—H12	0.9300
N3—C15	1.353 (4)	C13—C14	1.376 (6)
N4—C20	1.338 (4)	C13—H13	0.9300
N4—C16	1.344 (4)	C14—C15	1.382 (5)
N5—N6	1.202 (4)	C14—H14	0.9300
N6—N7	1.158 (4)	C15—C16	1.463 (5)
N8—N9	1.198 (4)	C16—C17	1.385 (5)
N9—N10	1.151 (5)	C17—C18	1.375 (6)
C1—C2	1.372 (5)	C17—H17	0.9300
C1—H1	0.9300	C18—C19	1.365 (6)
C2—C3	1.368 (6)	C18—H18	0.9300
C2—H2	0.9300	C19—C20	1.375 (5)
C3—C4	1.385 (6)	C19—H19	0.9300
C3—H3	0.9300	C20—H20	0.9300

O3—Cl1—O2	111.4 (5)	N2—C5—C4	121.5 (3)
O3—Cl1—O4	105.3 (6)	N2—C5—C6	113.7 (3)
O2—Cl1—O4	110.4 (5)	C4—C5—C6	124.8 (3)
O3—Cl1—O1	112.7 (5)	N1—C6—C7	121.7 (3)
O2—Cl1—O1	109.1 (3)	N1—C6—C5	113.7 (3)
O4—Cl1—O1	107.8 (4)	C7—C6—C5	124.6 (3)
N1—Co1—N4	178.80 (11)	C6—C7—C8	119.1 (4)
N1—Co1—N8	91.71 (12)	C6—C7—H7	120.4
N4—Co1—N8	88.34 (12)	C8—C7—H7	120.4
N1—Co1—N5	88.79 (12)	C9—C8—C7	119.2 (4)
N4—Co1—N5	92.41 (12)	C9—C8—H8	120.4
N8—Co1—N5	92.31 (13)	C7—C8—H8	120.4
N1—Co1—N3	96.30 (12)	C8—C9—C10	119.4 (4)
N4—Co1—N3	82.50 (12)	C8—C9—H9	120.3
N8—Co1—N3	87.51 (12)	C10—C9—H9	120.3
N5—Co1—N3	174.91 (12)	N1—C10—C9	121.7 (4)
N1—Co1—N2	82.47 (12)	N1—C10—H10	119.1
N4—Co1—N2	97.44 (12)	C9—C10—H10	119.1
N8—Co1—N2	173.90 (12)	N3—C11—C12	122.3 (4)
N5—Co1—N2	89.40 (12)	N3—C11—H11	118.8
N3—Co1—N2	91.30 (12)	C12—C11—H11	118.8
C10—N1—C6	118.9 (3)	C11—C12—C13	119.4 (4)
C10—N1—Co1	125.7 (3)	C11—C12—H12	120.3
C6—N1—Co1	115.3 (2)	C13—C12—H12	120.3
C1—N2—C5	118.7 (3)	C12—C13—C14	118.8 (4)
C1—N2—Co1	126.5 (3)	C12—C13—H13	120.6
C5—N2—Co1	114.8 (2)	C14—C13—H13	120.6
C11—N3—C15	118.8 (3)	C13—C14—C15	119.8 (4)
C11—N3—Co1	127.1 (2)	C13—C14—H14	120.1
C15—N3—Co1	114.1 (2)	C15—C14—H14	120.1
C20—N4—C16	119.1 (3)	N3—C15—C14	120.8 (3)
C20—N4—Co1	126.0 (2)	N3—C15—C16	113.9 (3)
C16—N4—Co1	114.3 (2)	C14—C15—C16	125.3 (3)
N6—N5—Co1	116.5 (2)	N4—C16—C17	121.1 (3)
N7—N6—N5	177.0 (4)	N4—C16—C15	114.2 (3)
N9—N8—Co1	117.8 (2)	C17—C16—C15	124.7 (3)
N10—N9—N8	176.2 (4)	C18—C17—C16	119.1 (4)
N2—C1—C2	121.8 (4)	C18—C17—H17	120.4
N2—C1—H1	119.1	C16—C17—H17	120.4
C2—C1—H1	119.1	C19—C18—C17	119.5 (4)
C3—C2—C1	119.9 (4)	C19—C18—H18	120.3
C3—C2—H2	120.0	C17—C18—H18	120.3
C1—C2—H2	120.0	C18—C19—C20	119.1 (4)
C2—C3—C4	118.9 (4)	C18—C19—H19	120.5
C2—C3—H3	120.5	C20—C19—H19	120.5
C4—C3—H3	120.5	N4—C20—C19	122.1 (4)
C5—C4—C3	119.1 (4)	N4—C20—H20	119.0
C5—C4—H4	120.4	C19—C20—H20	119.0
C3—C4—H4	120.4		

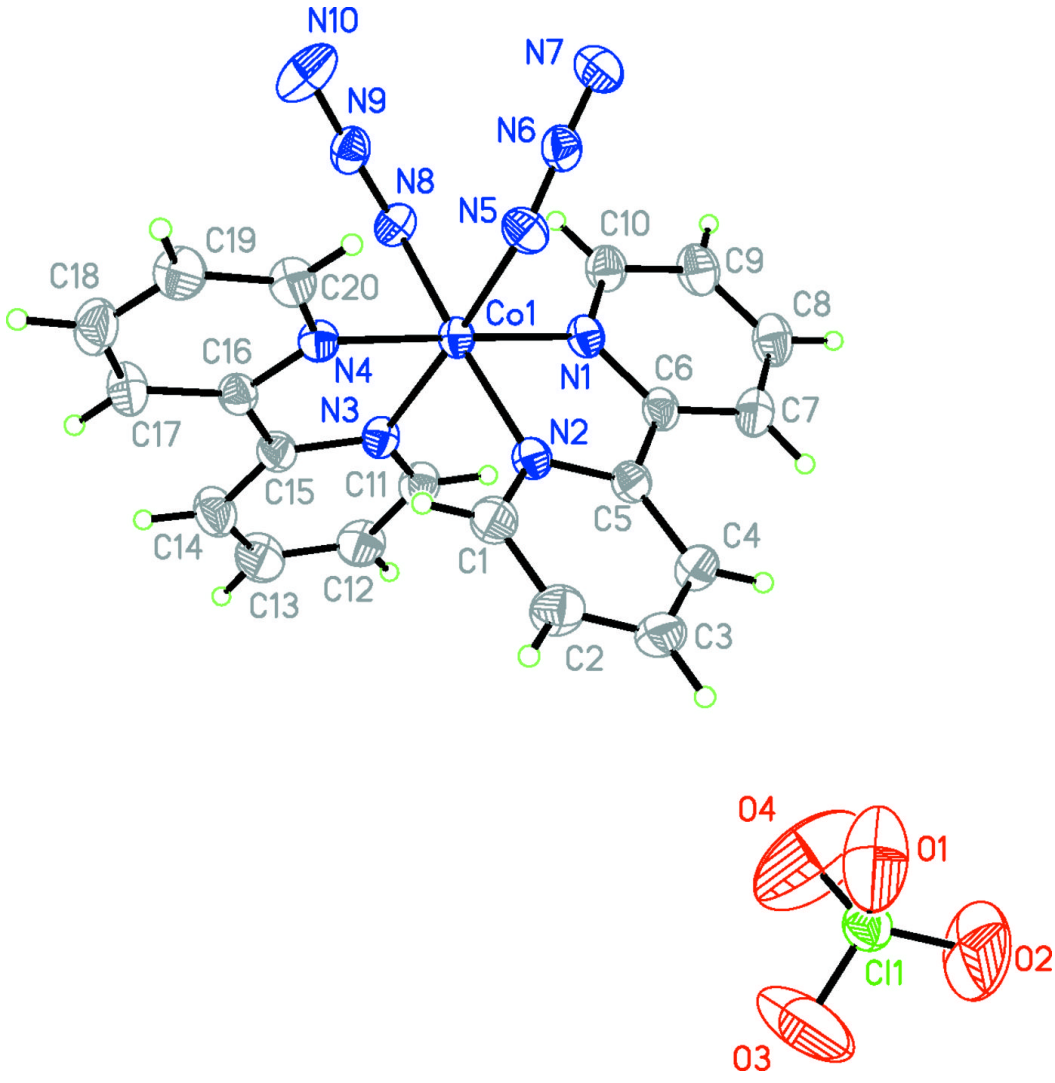
N8—Co1—N1—C10	5.9 (3)	Co1—N2—C5—C4	−179.5 (3)
N5—Co1—N1—C10	−86.3 (3)	C1—N2—C5—C6	−177.2 (3)
N3—Co1—N1—C10	93.6 (3)	Co1—N2—C5—C6	2.0 (4)
N2—Co1—N1—C10	−175.9 (3)	C3—C4—C5—N2	−0.5 (6)
N8—Co1—N1—C6	−178.4 (2)	C3—C4—C5—C6	177.8 (3)
N5—Co1—N1—C6	89.3 (2)	C10—N1—C6—C7	−0.4 (5)
N3—Co1—N1—C6	−90.7 (2)	Co1—N1—C6—C7	−176.3 (3)
N2—Co1—N1—C6	−0.3 (2)	C10—N1—C6—C5	177.3 (3)
N1—Co1—N2—C1	178.1 (3)	Co1—N1—C6—C5	1.4 (4)
N4—Co1—N2—C1	−3.1 (3)	N2—C5—C6—N1	−2.2 (4)
N5—Co1—N2—C1	89.3 (3)	C4—C5—C6—N1	179.4 (3)
N3—Co1—N2—C1	−85.7 (3)	N2—C5—C6—C7	175.4 (3)
N1—Co1—N2—C5	−1.0 (2)	C4—C5—C6—C7	−3.0 (6)
N4—Co1—N2—C5	177.8 (2)	N1—C6—C7—C8	1.2 (5)
N5—Co1—N2—C5	−89.9 (2)	C5—C6—C7—C8	−176.2 (3)
N3—Co1—N2—C5	95.2 (2)	C6—C7—C8—C9	−1.2 (6)
N1—Co1—N3—C11	4.0 (3)	C7—C8—C9—C10	0.4 (6)
N4—Co1—N3—C11	−175.9 (3)	C6—N1—C10—C9	−0.5 (5)
N8—Co1—N3—C11	95.5 (3)	Co1—N1—C10—C9	175.0 (3)
N2—Co1—N3—C11	−78.6 (3)	C8—C9—C10—N1	0.5 (6)
N1—Co1—N3—C15	−172.9 (2)	C15—N3—C11—C12	0.6 (6)
N4—Co1—N3—C15	7.2 (2)	Co1—N3—C11—C12	−176.3 (3)
N8—Co1—N3—C15	−81.5 (3)	N3—C11—C12—C13	0.1 (7)
N2—Co1—N3—C15	104.5 (3)	C11—C12—C13—C14	0.1 (7)
N8—Co1—N4—C20	−92.5 (3)	C12—C13—C14—C15	−0.9 (7)
N5—Co1—N4—C20	−0.2 (3)	C11—N3—C15—C14	−1.4 (5)
N3—Co1—N4—C20	179.8 (3)	Co1—N3—C15—C14	175.9 (3)
N2—Co1—N4—C20	89.5 (3)	C11—N3—C15—C16	179.0 (3)
N8—Co1—N4—C16	78.2 (2)	Co1—N3—C15—C16	−3.7 (4)
N5—Co1—N4—C16	170.4 (2)	C13—C14—C15—N3	1.5 (6)
N3—Co1—N4—C16	−9.5 (2)	C13—C14—C15—C16	−178.9 (4)
N2—Co1—N4—C16	−99.9 (2)	C20—N4—C16—C17	2.0 (5)
N1—Co1—N5—N6	53.8 (3)	Co1—N4—C16—C17	−169.3 (3)
N4—Co1—N5—N6	−126.3 (3)	C20—N4—C16—C15	−178.6 (3)
N8—Co1—N5—N6	−37.8 (3)	Co1—N4—C16—C15	10.0 (4)
N2—Co1—N5—N6	136.3 (3)	N3—C15—C16—N4	−4.1 (5)
N1—Co1—N8—N9	−134.8 (3)	C14—C15—C16—N4	176.3 (4)
N4—Co1—N8—N9	46.4 (3)	N3—C15—C16—C17	175.2 (3)
N5—Co1—N8—N9	−46.0 (3)	C14—C15—C16—C17	−4.4 (6)
N3—Co1—N8—N9	129.0 (3)	N4—C16—C17—C18	−0.3 (6)
C5—N2—C1—C2	−0.9 (5)	C15—C16—C17—C18	−179.5 (4)
Co1—N2—C1—C2	180.0 (3)	C16—C17—C18—C19	−1.9 (6)
N2—C1—C2—C3	−0.2 (6)	C17—C18—C19—C20	2.2 (6)
C1—C2—C3—C4	1.0 (6)	C16—N4—C20—C19	−1.7 (5)
C2—C3—C4—C5	−0.6 (6)	Co1—N4—C20—C19	168.6 (3)
C1—N2—C5—C4	1.2 (5)	C18—C19—C20—N4	−0.5 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···N8	0.93	2.38	2.906 (5)	115
C11—H11···N10^{i}	0.93	2.36	3.142 (6)	141
C13—H13···O2^{ii}	0.93	2.56	3.322 (6)	139
C14—H14···O1^{iii}	0.93	2.46	3.305 (6)	152
C17—H17···O1^{iii}	0.93	2.55	3.430 (6)	157
C18—H18···O1^{iv}	0.93	2.47	3.326 (6)	154
C20—H20···N5	0.93	2.43	2.938 (5)	114

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

Fig. 1


N10
N9
N8
N7
N6
N5
C19
C18
C20
C10
C9
C8
Co1
C16
N4
N1
C6
C7
N3
N2
C17
C15
C11
C5
C4
C14
C1
C12
C13
C2
C3
O4
O1
Cl1
O2
O3