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Bis(1,10-phenanthroline-κ^2N,N')-bis(cyanido-κC)cobalt(III) bis(azido-κ^1N)[1,2-bis(pyridine-2-carboxamido)-benzene-κ^4N]chromate(III) monohydrate

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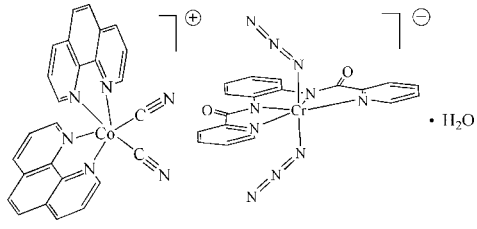
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.055; wR factor = 0.162; data-to-parameter ratio = 13.2.

The structure of the title compound, $[Co(C_{12}H_8N_2)_2(CN)_2]$-$[Cr(C_{18}H_{12}N_4O_2)(N_3)_2]\cdot H_2O$, comprises a $[Co^{III}(phen)_2(CN)_2]^+$ (phen = 1,10-phenanthroline) cation, a $[Cr^{III}(bpb)(N_3)_2]^-$ [bpb^{2-} = 1,2-bis(pyridine-2-carboxamido)benzene] anion and an uncoordinated water molecule. The Co and Cr ions are six-coordinated by N_4C_2 and N_6 sets, respectively, yielding distorted octahedral coordination geometries. The $[Co^{III}(phen)_2(CN)_2]^+$ and $[Cr^{III}(bpb)(N_3)_2]^-$ ions and water molecules are connected by π–π interactions [shortest distance 3.376 (2) Å] and O—H···O, O—H···N, C—H···O and C—H···N hydrogen bonds into a three-dimensional supramolecular network structure.

Related literature

For monomeric complexes with the ligand bpb^{2-}, see Ni *et al.* (2006); Che *et al.* (1988); for $[Co^{III}(bpb)(Et)(H_2O)]$ see Mak *et al.* (1991); Yang *et al.* (1991); and Dutta *et al.* (2000). For monomeric compounds containing two phen ligands and two cyanide groups, see Jian *et al.* (2004) and Zhan *et al.* (1996). For the synthesis of the precursor of (I), see Ni *et al.* (2005) and Zhong *et al.* (2006).



Experimental

Crystal data

$[Co(C_{12}H_8N_2)_2(CN)_2]$-$[Cr(C_{18}H_{12}N_4O_2)(N_3)_2]\cdot H_2O$
M_r = 941.77
Monoclinic, $P2_1/c$
a = 12.488 (3) Å
b = 20.633 (4) Å
c = 16.152 (3) Å
β = 105.51 (3)°
V = 4010.2 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 293 (2) K
0.12 × 0.08 × 0.06 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.932, T_{max} = 0.955
14094 measured reflections
7868 independent reflections
6341 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.162
S = 1.08
7868 reflections
594 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O1	0.85	2.08	2.919 (2)	171
O1W—H1B···N2^{i}	0.85	2.37	3.095 (2)	143
C4—H4···N1^{ii}	0.93	2.39	3.194 (5)	144
C21—H21···N5^{iii}	0.93	2.50	3.158 (6)	128
C22—H22···N5^{iii}	0.93	2.68	3.239 (6)	120
C23—H23···O1W^{iii}	0.93	2.62	3.268 (2)	128
C26—H26···N3^{iv}	0.93	2.45	3.240 (5)	143
C30—H30···O1^{i}	0.93	2.45	3.177 (3)	135
C33—H33···N8^{i}	0.93	2.44	3.223 (6)	142
C38—H38···N6^{v}	0.93	2.50	3.241 (5)	137
C42—H42···O1W	0.93	2.53	3.327 (2)	144

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL97* and *XP*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2289).

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supplementary materials

Acta Cryst. (2007). E**63**, m2531-m2532 [**doi:10.1107/S1600536807043693**]

Bis(1,10-phenanthroline-κ^2N,N')-bis(cyanido-κC)cobalt(III) bis(azido-κ^1N)[1,2-bis(pyridine-2-carboxamido)benzene-κ^4N]chromate(III) monohydrate

Z.-H. Ni

Comment

The crystal structures of the monomeric complexes [Cr(bpb)(H_2O)(OH)] and [Cr(bpb)(H_2O)(N_3)] (Ni *et al.*, 2006), [Cr^V(bpb)(N)] (Che *et al.*, 1988), [Co^{III}(bpb)(Et)(H_2O)] (Mak *et al.*, 1991), (Et_3HN)[Fe^{III}(bpb)($Cl)_2$]·CH_3CN (Yang *et al.*, 1991) and Na[Fe^{III}(bpb)($N_3)_2$] and Na[Fe^{III}(bpb)($CN)_2$] (Dutta *et al.*, 2000) contain a large in-plane pyridine carboxamide ligand bpb^{2-}.

The monomeric complexes [Co(phen)$_2$(CN)$_2$]·EtOH·H_2O (Jian *et al.*, 2004) and [Fe(phen)$_2$)(CN)$_2$]·3H_2O (Zhan *et al.*, 1996) show two phen ligands and two cyanide groups. Herein, we report a new ion-pair complex [Co^{III}(phen)$_2$(CN)$_2$][Cr^{III}(bpb)($N_3)_2$]·H_2O (I) containing a large in-plane pyridine carboxamide ligand bpb^{2-} and two phen ligands and two cyanide groups as well as two azide groups.

The geometry and labeling scheme for the crystal structure of the title complex are depicted in Figure 1. The title compound a $[Co^{III}(phen)_2(CN)_2]^+$ cation and a $[Cr^{III}(bpb)(N_3)_2]^-$ anion as well as a free water molecule. The Co(III) ion in the cation is coordinated by four nitrogen atoms from two *cis* phen ligands and two carbon atoms from two *cis* cyanide groups, giving a distorted octahedral coordination environment. The averaged Co—N_{phen} bond length is 1.970 (3) Å. The Co—$C_{cyanide}$ bond lengths are 1.913 (4)Å for Co—C1 and 1.891 (3) for Co—C2. The two phen molecules in $[Co^{III}(phen)_2(CN)_2]^+$ cation are nearly planar, and the two planes are almost vertical with a dihedral angle of 89.7 (1)°.

The Cr(III) ion in the anion unit $[Cr^{III}(bpb)(N_3)_2]^-$ is coordinated in the equatorial plane by a large in-plane bpb^{2-} ligand through two pyridine and two deprotonated carboxamide nitrogen atoms. The two *trans* positions were occupied by two azide groups. The ligand bpb^{2-}, two azide N atoms provide a six-coordination circumstance around Cr(III) center for $[Cr^{III}(bpb)(N_3)_2]^-$ unit. The C—O, $C_{pyridine}$—N, and $C_{carboxy}$—N bond distances from bpb^{2-} ligand in the title complex agree with those reported for other mononuclear complexes such as [Co^{III}(bpb)(Et)(H_2O)], $[Fe^{III}(bpb)(Cl)_2]^-$ and $[Fe^{III}(bpb)(CN)_2]^-$, which indicate these bond lengths do not vary much with the nature of central metal ion and their spin states. The average bond distances of Cr—N_{amide} and Cr—$N_{pyridine}$ are 1.989 (3) Å and 2.112 (3) Å, which is in agreement with the fact that the deprotonated amide group is a very strong σ-donor.

There exist hydrogen bonds involving free water molecule and carboxamide oxygen atoms and cyanide and azide nitrogen atoms (Table 1), and π-π interactions between phen and bpb^{2-} ligands with the shorest distance of 3.376 (2) Å, which link the [Co^{III}(phen)$_2$(CN)$_2$][Cr^{III}(bpb)($N_3)_2$]·H_2O (I) molecules into a three-dimensional supramolecular structure.

The formation mechanism of (I) is due to that $Na[Cr(bpb)(N_3)_2]$ and $[Cr(phen)_2(CN)_2]^+$ is more stable than precursor $Na[Cr(bpb)(CN)_2]$ in the reaction system. In addition, oxidation Co(II) is observed in this reaction system.

Experimental

$K[Cr(bpb)(CN)_2]$ was synthesized according to literature (Ni *et al.*, 2005). $[Co(phen)_2(Cl)_2]$ was synthesized according to literature (Zhong *et al.*, 2006). The title complex was prepared as follows. A methanol solution (5 ml) of $[Co(phen)_2(Cl)_2]$ (97 mg, 0.2 mmol) was added to a MeOH and H_2O solution (20 ml, MeOH/H_2O = 4:1 *v*/*v*) of $K[Cr(bpb)(CN)_2]$ (92 mg, 0.2 mmol). Then, an aqueous solution (5 ml) of NaN_3 (33 mg, 0.6 mmol) was added. The mixture was carefully filtered and the resulting solution was kept at room temperature for about two days, producing block brown crystals of (I).

Refinement

The coordinates of the H atoms of the water molecules were found from difference Fourier maps and normalized to O—H distances of 0.85 Å. H atoms bound to C atoms were placed using the HFIX commands in *SHELXL-97*, with C—H distances of 0.93 Å. All H atoms were allowed for as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$. A value for R_{int} could not be determined as data processing of the title complex was based on averaged intensities of diffraction spots.

Figures

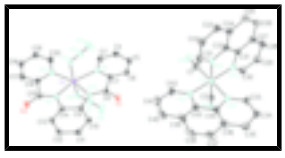

Fig. 1. A view of (I) with the unique atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level, solvate water molecules and all H atoms bonded to C atoms are omitted.

Fig. 2. A stereoview of part of the crystal structure of (I) along *a* axis, showing two-dimensional supramolecular structure through π-π interactions and hydrogen bonds.

Bis(1,10-phenanthroline-κ^2N,N')- bis(cyanido-κC)cobalt(III) bis(azido-κ^1N)[1,2-bis(pyridine-2-carboxamido)benzene- κ^4N]chromate(III) monohydrate

Crystal data

$[Co(C_{12}H_8N_2)_2(CN)_2][Cr(C_{18}H_{12}N_4O_2)(N_3)_2]\cdot H_2O$	F_{000} = 1924
M_r = 941.77	D_x = 1.560 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 7868 reflections
$a = 12.488$ (3) Å	$\theta = 3.1–26.0°$
$b = 20.633$ (4) Å	$\mu = 0.75$ mm^{-1}
$c = 16.152$ (3) Å	$T = 293$ (2) K
$\beta = 105.51$ (3)°	Block, brown
$V = 4010.2$ (14) Å^3	0.12 × 0.08 × 0.06 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector diffractometer	7868 independent reflections
Radiation source: fine-focus sealed tube	6341 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.046$
$T = 293(2)$ K	$\theta_{max} = 26.0°$
φ and ω scans	$\theta_{min} = 3.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -15\rightarrow15$
$T_{min} = 0.932$, $T_{max} = 0.955$	$k = -22\rightarrow25$
14094 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.162$	$w = 1/[\sigma^2(F_o^2) + (0.1216P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
7868 reflections	$\Delta\rho_{max} = 0.72$ e Å^{-3}
594 parameters	$\Delta\rho_{min} = -0.85$ 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 $F^2 > \sigma(F^2)$ 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}
Co	0.48482 (3)	0.43739 (2)	0.26435 (3)	0.03403 (15)
Cr	0.04038 (4)	0.31652 (2)	0.78682 (3)	0.02753 (14)
N16	0.4510 (2)	0.36270 (12)	0.18250 (16)	0.0355 (6)
N14	0.4596 (2)	0.49881 (12)	0.16649 (16)	0.0340 (6)
N13	0.3268 (2)	0.45023 (13)	0.25147 (18)	0.0387 (6)
N15	0.6384 (2)	0.42009 (12)	0.26441 (16)	0.0345 (6)
C2	0.5214 (3)	0.50586 (15)	0.3448 (2)	0.0363 (7)
C44	0.3497 (3)	0.51591 (15)	0.13662 (19)	0.0375 (7)
C31	0.6473 (2)	0.36849 (14)	0.21268 (18)	0.0320 (6)
C26	0.7494 (3)	0.29169 (16)	0.1469 (2)	0.0422 (8)
H26	0.8163	0.2768	0.1391	0.051*
C25	0.6524 (3)	0.26162 (16)	0.1057 (2)	0.0413 (7)
H25	0.6543	0.2262	0.0705	0.050*
C32	0.5461 (3)	0.33708 (14)	0.16906 (18)	0.0326 (6)
C27	0.7491 (3)	0.34638 (15)	0.2023 (2)	0.0375 (7)
C42	0.2629 (3)	0.42475 (17)	0.2973 (2)	0.0485 (9)
H42	0.2954	0.3999	0.3455	0.058*
C43	0.2782 (3)	0.48836 (16)	0.1827 (2)	0.0402 (7)
C33	0.5317 (3)	0.52480 (15)	0.1277 (2)	0.0378 (7)
H33	0.6066	0.5142	0.1475	0.045*
C30	0.7311 (3)	0.45073 (15)	0.3062 (2)	0.0381 (7)
H30	0.7261	0.4858	0.3412	0.046*
C39	0.1631 (3)	0.50154 (19)	0.1558 (2)	0.0497 (9)
C1	0.5089 (3)	0.38246 (17)	0.3630 (2)	0.0477 (8)
C36	0.3083 (3)	0.55698 (17)	0.0659 (2)	0.0455 (8)
C24	0.5466 (3)	0.28377 (15)	0.11573 (19)	0.0359 (7)
C34	0.4979 (3)	0.56720 (16)	0.0586 (2)	0.0442 (8)
H34	0.5502	0.5848	0.0335	0.053*
N2	0.5447 (2)	0.54653 (14)	0.39523 (18)	0.0439 (7)
C21	0.3543 (3)	0.33494 (17)	0.1426 (2)	0.0431 (8)
H21	0.2891	0.3517	0.1514	0.052*
C22	0.3479 (3)	0.28153 (17)	0.0882 (2)	0.0457 (8)
H22	0.2790	0.2637	0.0614	0.055*
C23	0.4426 (3)	0.25524 (16)	0.0740 (2)	0.0428 (8)
H23	0.4387	0.2196	0.0380	0.051*
C28	0.8464 (3)	0.37959 (16)	0.2482 (2)	0.0442 (8)
H28	0.9159	0.3664	0.2439	0.053*
C29	0.8367 (3)	0.43134 (17)	0.2990 (2)	0.0471 (8)
H29	0.8999	0.4538	0.3287	0.057*
C40	0.0974 (3)	0.4723 (2)	0.2051 (3)	0.0601 (11)
H40	0.0209	0.4787	0.1904	0.072*
C41	0.1474 (3)	0.4346 (2)	0.2741 (3)	0.0568 (10)
H41	0.1044	0.4153	0.3063	0.068*
C35	0.3872 (3)	0.58321 (17)	0.0271 (2)	0.0484 (8)
H35	0.3647	0.6112	−0.0195	0.058*

N1	0.5321 (3)	0.35124 (16)	0.4228 (2)	0.0646 (10)
C37	0.1908 (3)	0.5694 (2)	0.0390 (2)	0.0575 (10)
H37	0.1616	0.5957	−0.0084	0.069*
C38	0.1223 (3)	0.5429 (2)	0.0825 (3)	0.0594 (11)
H38	0.0466	0.5518	0.0642	0.071*
O1	0.16269 (17)	0.41625 (10)	0.61221 (13)	0.0341 (5)
N10	0.04882 (19)	0.37818 (11)	0.69427 (15)	0.0287 (5)
N9	0.2114 (2)	0.30820 (11)	0.79160 (16)	0.0318 (5)
C14	−0.1470 (2)	0.38842 (13)	0.68146 (17)	0.0285 (6)
C9	−0.0538 (2)	0.40809 (14)	0.65158 (18)	0.0284 (6)
C7	0.2385 (2)	0.34648 (13)	0.73176 (18)	0.0293 (6)
O2	−0.28973 (18)	0.33717 (12)	0.78485 (15)	0.0425 (5)
N3	0.0139 (2)	0.23662 (13)	0.71132 (18)	0.0389 (6)
C10	−0.0714 (2)	0.45191 (13)	0.58276 (18)	0.0303 (6)
H10	−0.0118	0.4658	0.5630	0.036*
N12	−0.0250 (2)	0.26168 (12)	0.87107 (15)	0.0326 (5)
N11	−0.11798 (19)	0.34461 (12)	0.75174 (15)	0.0298 (5)
C8	0.1444 (2)	0.38425 (13)	0.67296 (18)	0.0296 (6)
C13	−0.2535 (2)	0.41110 (15)	0.64024 (19)	0.0335 (6)
H13	−0.3141	0.3974	0.6589	0.040*
N6	0.0900 (2)	0.38274 (14)	0.88251 (17)	0.0421 (6)
N4	0.0581 (2)	0.21842 (14)	0.65907 (18)	0.0432 (7)
C15	−0.1905 (2)	0.32277 (15)	0.79499 (19)	0.0333 (6)
C6	0.3468 (3)	0.35121 (15)	0.72515 (19)	0.0350 (7)
H6	0.3631	0.3771	0.6830	0.042*
C3	0.2934 (3)	0.27424 (16)	0.8455 (2)	0.0393 (7)
H3	0.2752	0.2471	0.8857	0.047*
C16	−0.1345 (2)	0.27401 (14)	0.86214 (18)	0.0336 (6)
N7	0.1550 (3)	0.42476 (17)	0.8833 (2)	0.0571 (9)
C17	−0.1936 (3)	0.24049 (17)	0.9103 (2)	0.0422 (8)
H17	−0.2683	0.2496	0.9041	0.051*
C5	0.4312 (3)	0.31656 (15)	0.7828 (2)	0.0381 (7)
H5	0.5045	0.3196	0.7799	0.046*
C4	0.4039 (3)	0.27792 (16)	0.8437 (2)	0.0422 (8)
H4	0.4585	0.2547	0.8830	0.051*
C20	0.0263 (3)	0.21634 (16)	0.9270 (2)	0.0408 (7)
H20	0.1013	0.2084	0.9330	0.049*
C19	−0.0279 (3)	0.18087 (17)	0.9763 (2)	0.0450 (8)
H19	0.0097	0.1495	1.0144	0.054*
C18	−0.1399 (3)	0.19328 (17)	0.9675 (2)	0.0460 (8)
H18	−0.1784	0.1701	0.9997	0.055*
N5	0.0992 (4)	0.1979 (2)	0.6088 (3)	0.0848 (13)
N8	0.2144 (4)	0.4691 (2)	0.8828 (3)	0.1045 (18)
O1W	0.2765 (2)	0.36408 (11)	0.49069 (15)	0.0454 (5)
C11	−0.1783 (3)	0.47473 (15)	0.54393 (18)	0.0346 (7)
H11	−0.1890	0.5042	0.4989	0.042*
C12	−0.2696 (3)	0.45383 (15)	0.57176 (19)	0.0369 (7)
H12	−0.3406	0.4685	0.5444	0.044*
H1A	0.2384	0.3754	0.5245	0.055*

H1B	0.3419	0.3797	0.5070	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0382 (3)	0.0328 (2)	0.0358 (2)	−0.00662 (17)	0.01811 (18)	−0.00425 (17)
Cr	0.0251 (2)	0.0305 (3)	0.0292 (2)	−0.00140 (17)	0.01109 (18)	0.00460 (18)
N16	0.0385 (14)	0.0345 (13)	0.0386 (13)	−0.0076 (11)	0.0190 (11)	−0.0037 (11)
N14	0.0363 (14)	0.0340 (13)	0.0362 (13)	−0.0057 (11)	0.0172 (11)	−0.0071 (11)
N13	0.0411 (15)	0.0392 (14)	0.0408 (14)	−0.0081 (12)	0.0196 (12)	−0.0100 (12)
N15	0.0372 (14)	0.0311 (13)	0.0360 (13)	−0.0010 (11)	0.0110 (11)	−0.0017 (11)
C2	0.0354 (16)	0.0374 (17)	0.0406 (16)	−0.0035 (13)	0.0179 (13)	−0.0024 (14)
C44	0.0414 (17)	0.0373 (17)	0.0373 (16)	0.0017 (14)	0.0163 (13)	−0.0095 (13)
C31	0.0371 (16)	0.0285 (14)	0.0319 (14)	0.0027 (12)	0.0119 (12)	0.0022 (12)
C26	0.0405 (18)	0.0386 (17)	0.0471 (18)	0.0119 (14)	0.0108 (14)	−0.0020 (15)
C25	0.0492 (19)	0.0315 (16)	0.0421 (17)	0.0089 (14)	0.0103 (14)	−0.0022 (13)
C32	0.0386 (16)	0.0311 (15)	0.0307 (14)	−0.0013 (12)	0.0135 (12)	0.0003 (12)
C27	0.0359 (17)	0.0321 (16)	0.0421 (17)	0.0058 (13)	0.0062 (13)	0.0023 (13)
C42	0.060 (2)	0.0448 (19)	0.052 (2)	−0.0142 (16)	0.0351 (18)	−0.0120 (16)
C43	0.0412 (17)	0.0460 (18)	0.0397 (17)	−0.0044 (14)	0.0219 (14)	−0.0168 (14)
C33	0.0409 (17)	0.0364 (16)	0.0409 (17)	−0.0079 (13)	0.0190 (14)	−0.0041 (14)
C30	0.0363 (17)	0.0360 (16)	0.0406 (17)	−0.0036 (13)	0.0079 (13)	−0.0056 (13)
C39	0.0413 (19)	0.058 (2)	0.054 (2)	0.0003 (16)	0.0204 (16)	−0.0227 (18)
C1	0.063 (2)	0.0397 (19)	0.047 (2)	−0.0150 (16)	0.0257 (17)	−0.0051 (16)
C36	0.053 (2)	0.0433 (19)	0.0416 (18)	0.0054 (16)	0.0148 (15)	−0.0090 (15)
C24	0.0448 (18)	0.0330 (16)	0.0309 (14)	−0.0031 (13)	0.0117 (13)	0.0001 (12)
C34	0.058 (2)	0.0417 (18)	0.0406 (18)	−0.0042 (16)	0.0269 (16)	−0.0042 (15)
N2	0.0464 (17)	0.0456 (16)	0.0440 (16)	−0.0035 (13)	0.0197 (13)	−0.0026 (14)
C21	0.0381 (18)	0.0483 (19)	0.0466 (19)	−0.0076 (15)	0.0176 (15)	−0.0053 (16)
C22	0.0455 (19)	0.048 (2)	0.0469 (18)	−0.0153 (16)	0.0173 (15)	−0.0131 (16)
C23	0.056 (2)	0.0361 (17)	0.0396 (17)	−0.0096 (15)	0.0184 (15)	−0.0060 (14)
C28	0.0334 (17)	0.0446 (19)	0.0526 (19)	0.0062 (14)	0.0078 (14)	−0.0045 (15)
C29	0.0375 (18)	0.046 (2)	0.055 (2)	−0.0030 (15)	0.0063 (16)	−0.0113 (16)
C40	0.0376 (19)	0.073 (3)	0.076 (3)	−0.0107 (19)	0.0267 (19)	−0.038 (2)
C41	0.054 (2)	0.060 (2)	0.067 (3)	−0.0208 (19)	0.035 (2)	−0.024 (2)
C35	0.070 (2)	0.0411 (18)	0.0382 (17)	0.0057 (17)	0.0218 (17)	−0.0002 (15)
N1	0.093 (3)	0.0475 (19)	0.0525 (19)	−0.0193 (18)	0.0174 (18)	−0.0004 (16)
C37	0.056 (2)	0.069 (3)	0.046 (2)	0.021 (2)	0.0112 (18)	−0.0079 (18)
C38	0.0367 (19)	0.077 (3)	0.063 (2)	0.0106 (18)	0.0106 (17)	−0.027 (2)
O1	0.0360 (11)	0.0369 (11)	0.0349 (11)	−0.0014 (9)	0.0189 (9)	0.0054 (9)
N10	0.0267 (12)	0.0304 (12)	0.0309 (12)	−0.0008 (9)	0.0110 (9)	0.0023 (10)
N9	0.0294 (13)	0.0319 (13)	0.0352 (13)	−0.0026 (10)	0.0106 (10)	0.0033 (10)
C14	0.0329 (15)	0.0298 (14)	0.0252 (13)	0.0008 (12)	0.0120 (11)	−0.0017 (11)
C9	0.0310 (15)	0.0281 (14)	0.0294 (13)	0.0021 (11)	0.0134 (11)	−0.0017 (11)
C7	0.0278 (14)	0.0268 (14)	0.0343 (14)	−0.0040 (11)	0.0101 (11)	−0.0023 (12)
O2	0.0334 (12)	0.0527 (13)	0.0472 (13)	0.0067 (10)	0.0208 (10)	0.0123 (11)
N3	0.0340 (14)	0.0373 (14)	0.0526 (16)	−0.0067 (11)	0.0243 (12)	−0.0050 (12)
C10	0.0366 (16)	0.0276 (14)	0.0305 (14)	0.0016 (12)	0.0153 (12)	−0.0005 (12)

N12	0.0307 (13)	0.0356 (13)	0.0328 (12)	−0.0024 (10)	0.0106 (10)	0.0048 (11)
N11	0.0288 (12)	0.0320 (13)	0.0306 (12)	−0.0002 (10)	0.0113 (10)	0.0053 (10)
C8	0.0337 (15)	0.0272 (14)	0.0303 (14)	−0.0039 (12)	0.0129 (11)	−0.0007 (11)
C13	0.0293 (15)	0.0373 (16)	0.0352 (15)	0.0010 (12)	0.0109 (12)	−0.0018 (13)
N6	0.0441 (16)	0.0480 (16)	0.0390 (14)	−0.0097 (13)	0.0194 (12)	−0.0063 (12)
N4	0.0390 (15)	0.0460 (16)	0.0477 (16)	0.0054 (12)	0.0170 (13)	0.0062 (13)
C15	0.0300 (15)	0.0383 (16)	0.0339 (15)	−0.0003 (12)	0.0128 (12)	−0.0004 (12)
C6	0.0365 (16)	0.0349 (16)	0.0377 (15)	−0.0053 (13)	0.0173 (13)	−0.0011 (13)
C3	0.0351 (17)	0.0405 (18)	0.0425 (17)	0.0016 (13)	0.0104 (13)	0.0080 (14)
C16	0.0352 (16)	0.0359 (16)	0.0331 (15)	−0.0024 (13)	0.0148 (12)	0.0030 (12)
N7	0.0446 (17)	0.071 (2)	0.065 (2)	−0.0131 (17)	0.0302 (15)	−0.0287 (17)
C17	0.0376 (18)	0.050 (2)	0.0448 (18)	0.0018 (14)	0.0212 (14)	0.0090 (15)
C5	0.0278 (15)	0.0432 (18)	0.0456 (17)	−0.0015 (13)	0.0135 (13)	−0.0069 (14)
C4	0.0361 (17)	0.0414 (18)	0.0469 (18)	0.0063 (14)	0.0073 (14)	0.0031 (15)
C20	0.0374 (17)	0.0465 (19)	0.0399 (16)	−0.0008 (14)	0.0128 (14)	0.0102 (15)
C19	0.049 (2)	0.0461 (19)	0.0403 (17)	−0.0002 (15)	0.0119 (15)	0.0161 (15)
C18	0.050 (2)	0.049 (2)	0.0466 (19)	−0.0047 (15)	0.0276 (16)	0.0150 (16)
N5	0.089 (3)	0.112 (3)	0.069 (2)	0.039 (3)	0.048 (2)	0.004 (2)
N8	0.093 (3)	0.113 (4)	0.136 (4)	−0.061 (3)	0.079 (3)	−0.073 (3)
O1W	0.0485 (14)	0.0441 (13)	0.0477 (13)	0.0022 (11)	0.0203 (11)	−0.0017 (10)
C11	0.0463 (18)	0.0303 (15)	0.0280 (14)	0.0059 (13)	0.0113 (12)	0.0036 (12)
C12	0.0377 (17)	0.0380 (17)	0.0356 (16)	0.0071 (13)	0.0107 (13)	−0.0018 (13)

Geometric parameters (Å, °)

Co—C2	1.891 (3)	C28—H28	0.9300
Co—C1	1.913 (4)	C29—H29	0.9300
Co—N13	1.946 (3)	C40—C41	1.366 (6)
Co—N15	1.951 (3)	C40—H40	0.9300
Co—N14	1.984 (3)	C41—H41	0.9300
Co—N16	2.001 (3)	C35—H35	0.9300
Cr—N10	1.987 (2)	C37—C38	1.359 (6)
Cr—N11	1.992 (2)	C37—H37	0.9300
Cr—N3	2.024 (3)	C38—H38	0.9300
Cr—N6	2.032 (3)	O1—C8	1.254 (3)
Cr—N12	2.096 (2)	N10—C8	1.333 (4)
Cr—N9	2.123 (3)	N10—C9	1.423 (4)
N16—C21	1.336 (4)	N9—C3	1.350 (4)
N16—C32	1.370 (4)	N9—C7	1.359 (4)
N14—C33	1.340 (4)	C14—C13	1.399 (4)
N14—C44	1.373 (4)	C14—N11	1.420 (4)
N13—C42	1.333 (4)	C14—C9	1.433 (4)
N13—C43	1.364 (4)	C9—C10	1.404 (4)
N15—C30	1.333 (4)	C7—C6	1.388 (4)
N15—C31	1.376 (4)	C7—C8	1.514 (4)
C2—N2	1.152 (4)	O2—C15	1.242 (4)
C44—C36	1.405 (5)	N3—N4	1.187 (4)
C44—C43	1.426 (4)	C10—C11	1.396 (4)
C31—C27	1.402 (4)	C10—H10	0.9300

C31—C32	1.427 (4)	N12—C20	1.339 (4)
C26—C25	1.366 (5)	N12—C16	1.360 (4)
C26—C27	1.441 (4)	N11—C15	1.360 (4)
C26—H26	0.9300	C13—C12	1.387 (4)
C25—C24	1.447 (5)	C13—H13	0.9300
C25—H25	0.9300	N6—N7	1.186 (4)
C32—C24	1.398 (4)	N4—N5	1.152 (4)
C27—C28	1.420 (4)	C15—C16	1.507 (4)
C42—C41	1.405 (6)	C6—C5	1.402 (4)
C42—H42	0.9300	C6—H6	0.9300
C43—C39	1.411 (5)	C3—C4	1.389 (5)
C33—C34	1.392 (5)	C3—H3	0.9300
C33—H33	0.9300	C16—C17	1.392 (4)
C30—C29	1.413 (5)	N7—N8	1.179 (5)
C30—H30	0.9300	C17—C18	1.386 (5)
C39—C40	1.422 (6)	C17—H17	0.9300
C39—C38	1.439 (6)	C5—C4	1.379 (5)
C1—N1	1.132 (5)	C5—H5	0.9300
C36—C35	1.409 (5)	C4—H4	0.9300
C36—C37	1.438 (5)	C20—C19	1.384 (4)
C24—C23	1.422 (4)	C20—H20	0.9300
C34—C35	1.380 (5)	C19—C18	1.392 (5)
C34—H34	0.9300	C19—H19	0.9300
C21—C22	1.398 (5)	C18—H18	0.9300
C21—H21	0.9300	O1W—H1A	0.8472
C22—C23	1.375 (5)	O1W—H1B	0.8517
C22—H22	0.9300	C11—C12	1.401 (4)
C23—H23	0.9300	C11—H11	0.9300
C28—C29	1.371 (5)	C12—H12	0.9300
C2—Co—C1	85.12 (14)	C24—C23—H23	120.8
C2—Co—N13	91.34 (12)	C29—C28—C27	119.2 (3)
C1—Co—N13	95.68 (14)	C29—C28—H28	120.4
C2—Co—N15	94.57 (12)	C27—C28—H28	120.4
C1—Co—N15	87.44 (14)	C28—C29—C30	120.3 (3)
N13—Co—N15	173.54 (11)	C28—C29—H29	119.9
C2—Co—N14	91.60 (12)	C30—C29—H29	119.9
C1—Co—N14	176.61 (12)	C41—C40—C39	119.5 (4)
N13—Co—N14	83.53 (11)	C41—C40—H40	120.2
N15—Co—N14	93.67 (11)	C39—C40—H40	120.2
C2—Co—N16	177.62 (13)	C40—C41—C42	120.8 (4)
C1—Co—N16	93.01 (13)	C40—C41—H41	119.6
N13—Co—N16	90.31 (11)	C42—C41—H41	119.6
N15—Co—N16	83.87 (11)	C34—C35—C36	119.6 (3)
N14—Co—N16	90.29 (10)	C34—C35—H35	120.2
N10—Cr—N11	81.26 (10)	C36—C35—H35	120.2
N10—Cr—N3	95.81 (10)	C38—C37—C36	120.3 (4)
N11—Cr—N3	94.33 (11)	C38—C37—H37	119.9
N10—Cr—N6	94.30 (11)	C36—C37—H37	119.9
N11—Cr—N6	95.64 (11)	C37—C38—C39	122.1 (3)

N3—Cr—N6	166.76 (12)	C37—C38—H38	119.0
N10—Cr—N12	160.45 (10)	C39—C38—H38	119.0
N11—Cr—N12	79.19 (10)	C8—N10—C9	125.9 (2)
N3—Cr—N12	85.53 (10)	C8—N10—Cr	119.05 (19)
N6—Cr—N12	87.81 (10)	C9—N10—Cr	114.84 (18)
N10—Cr—N9	79.86 (10)	C3—N9—C7	118.0 (3)
N11—Cr—N9	161.12 (10)	C3—N9—Cr	130.4 (2)
N3—Cr—N9	87.54 (10)	C7—N9—Cr	111.50 (19)
N6—Cr—N9	85.85 (11)	C13—C14—N11	126.9 (3)
N12—Cr—N9	119.69 (10)	C13—C14—C9	120.0 (3)
C21—N16—C32	117.9 (3)	N11—C14—C9	113.1 (2)
C21—N16—Co	130.7 (2)	C10—C9—N10	126.4 (3)
C32—N16—Co	111.3 (2)	C10—C9—C14	118.7 (3)
C33—N14—C44	117.8 (3)	N10—C9—C14	114.9 (2)
C33—N14—Co	130.2 (2)	N9—C7—C6	121.9 (3)
C44—N14—Co	112.0 (2)	N9—C7—C8	116.5 (2)
C42—N13—C43	118.4 (3)	C6—C7—C8	121.6 (3)
C42—N13—Co	128.9 (3)	N4—N3—Cr	130.8 (2)
C43—N13—Co	112.6 (2)	C11—C10—C9	120.1 (3)
C30—N15—C31	118.4 (3)	C11—C10—H10	120.0
C30—N15—Co	129.3 (2)	C9—C10—H10	120.0
C31—N15—Co	112.3 (2)	C20—N12—C16	119.3 (3)
N2—C2—Co	178.4 (3)	C20—N12—Cr	128.0 (2)
N14—C44—C36	123.8 (3)	C16—N12—Cr	112.65 (18)
N14—C44—C43	114.9 (3)	C15—N11—C14	124.0 (2)
C36—C44—C43	121.3 (3)	C15—N11—Cr	120.28 (19)
N15—C31—C27	123.2 (3)	C14—N11—Cr	115.74 (18)
N15—C31—C32	116.6 (3)	O1—C8—N10	128.0 (3)
C27—C31—C32	120.3 (3)	O1—C8—C7	119.2 (3)
C25—C26—C27	120.5 (3)	N10—C8—C7	112.8 (2)
C25—C26—H26	119.7	C12—C13—C14	120.6 (3)
C27—C26—H26	119.7	C12—C13—H13	119.7
C26—C25—C24	121.3 (3)	C14—C13—H13	119.7
C26—C25—H25	119.3	N7—N6—Cr	124.6 (2)
C24—C25—H25	119.3	N5—N4—N3	176.9 (4)
N16—C32—C24	123.3 (3)	O2—C15—N11	129.1 (3)
N16—C32—C31	115.9 (3)	O2—C15—C16	120.6 (3)
C24—C32—C31	120.8 (3)	N11—C15—C16	110.3 (2)
C31—C27—C28	117.3 (3)	C7—C6—C5	119.3 (3)
C31—C27—C26	118.9 (3)	C7—C6—H6	120.4
C28—C27—C26	123.9 (3)	C5—C6—H6	120.4
N13—C42—C41	121.4 (4)	N9—C3—C4	123.0 (3)
N13—C42—H42	119.3	N9—C3—H3	118.5
C41—C42—H42	119.3	C4—C3—H3	118.5
N13—C43—C39	123.9 (3)	N12—C16—C17	121.1 (3)
N13—C43—C44	116.7 (3)	N12—C16—C15	117.5 (2)
C39—C43—C44	119.4 (3)	C17—C16—C15	121.3 (3)
N14—C33—C34	121.9 (3)	N8—N7—N6	176.0 (5)
N14—C33—H33	119.0	C18—C17—C16	119.2 (3)

C34—C33—H33	119.0	C18—C17—H17	120.4
N15—C30—C29	121.8 (3)	C16—C17—H17	120.4
N15—C30—H30	119.1	C4—C5—C6	118.9 (3)
C29—C30—H30	119.1	C4—C5—H5	120.6
C43—C39—C40	116.0 (4)	C6—C5—H5	120.6
C43—C39—C38	118.4 (3)	C5—C4—C3	118.9 (3)
C40—C39—C38	125.6 (3)	C5—C4—H4	120.6
N1—C1—Co	174.4 (4)	C3—C4—H4	120.6
C44—C36—C35	116.4 (3)	N12—C20—C19	122.6 (3)
C44—C36—C37	118.5 (3)	N12—C20—H20	118.7
C35—C36—C37	125.1 (3)	C19—C20—H20	118.7
C32—C24—C23	117.6 (3)	C20—C19—C18	118.5 (3)
C32—C24—C25	118.2 (3)	C20—C19—H19	120.8
C23—C24—C25	124.2 (3)	C18—C19—H19	120.8
C35—C34—C33	120.4 (3)	C17—C18—C19	119.4 (3)
C35—C34—H34	119.8	C17—C18—H18	120.3
C33—C34—H34	119.8	C19—C18—H18	120.3
N16—C21—C22	122.2 (3)	H1A—O1W—H1B	110.7
N16—C21—H21	118.9	C10—C11—C12	121.0 (3)
C22—C21—H21	118.9	C10—C11—H11	119.5
C23—C22—C21	120.5 (3)	C12—C11—H11	119.5
C23—C22—H22	119.7	C13—C12—C11	119.7 (3)
C21—C22—H22	119.7	C13—C12—H12	120.1
C22—C23—C24	118.4 (3)	C11—C12—H12	120.1
C22—C23—H23	120.8		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O1	0.85	2.08	2.919 (2)	171
O1W—H1B···N2^{i}	0.85	2.37	3.095 (2)	143
C4—H4···N1^{ii}	0.93	2.39	3.194 (5)	144
C21—H21···N5^{iii}	0.93	2.50	3.158 (6)	128
C22—H22···N5^{iii}	0.93	2.68	3.239 (6)	120
C23—H23···O1W^{iii}	0.93	2.62	3.268 (2)	128
C26—H26···N3^{iv}	0.93	2.45	3.240 (5)	143
C30—H30···O1^{i}	0.93	2.45	3.177 (3)	135
C33—H33···N8^{i}	0.93	2.44	3.223 (6)	142
C38—H38···N6^{v}	0.93	2.50	3.241 (5)	137
C42—H42···O1W	0.93	2.53	3.327 (2)	144

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

Fig. 1

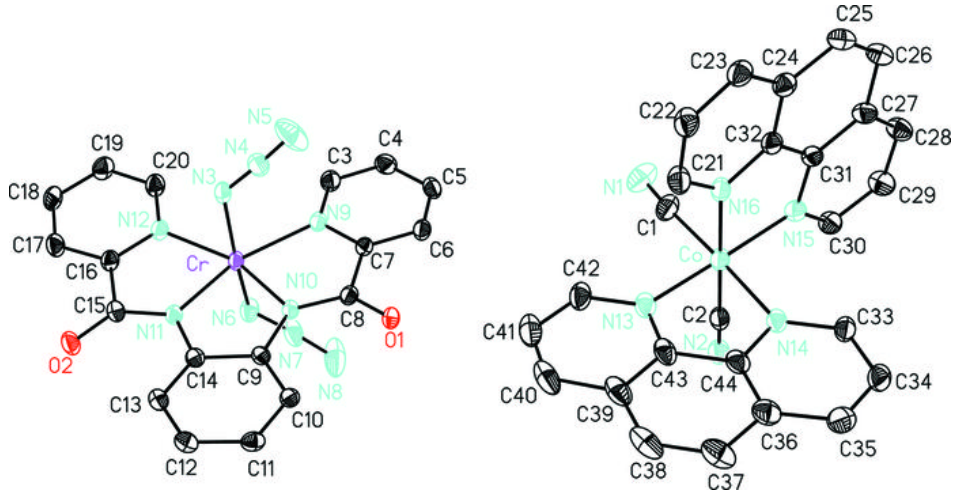
C25
C23
C24
C26
C22
C27
C32
C28
C21
C31
N1
C29
C1
N16
N15
C30
Co
C42
C2
C33
C41
N13
N2
N14
C43
C44
C34
C40
C39
C36
C35
C38
C37
C19
C20
N5
N4
N3
C3
C4
C5
C18
N12
N9
C17
C16
Cr
C7
C6
C15
N10
N6
C8
O1
N11
O2
N7
C14
C9
N8
C13
C10
C12
C11

Fig. 2