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Bis(cyanido-κC)bis(1,10-phenanthroline-κ^2N,N')chromium(III) bis(azido-κN)-[*N*,*N*′-(*o*-phenylene)bis(pyridine-2-carboxamide)-κ^4N]chromate(III) monohydrate

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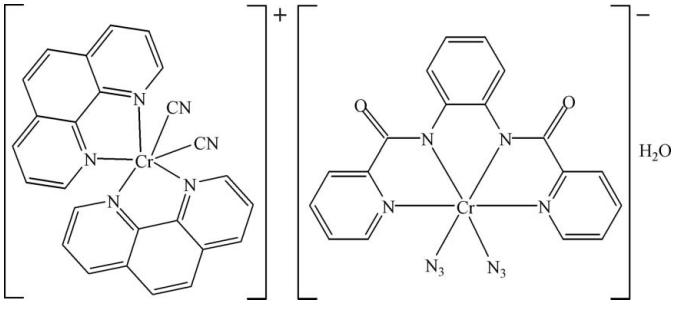
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.164; data-to-parameter ratio = 12.3.

The title compound, $[Cr(CN)_2(C_{12}H_8N_2)_2][Cr(N_3)_2(C_{18}H_{12}N_4O_2)]\cdot H_2O$, contains $[Cr^{III}(CN)_2(phen)_2]^+$ cations (phen is 1,10-phenanthroline) and $[Cr^{III}(N_3)_2(bpb)]^-$ anions [bpb is 1,2-bis(pyridine-2-carboxamido)benzene or *N*,*N*′-(*o*-phenylene)bis(pyridine-2-carboxamide)]. In the cations, the Cr^{III} atom is coordinated by two phen ligands and two cyanide ligands in a distorted octahedral geometry. In the anions, the Cr^{III} atom is coordinated by the tetradentate bpb ligand and two azide ions, forming a distorted octahedral geometry. There is one solvent water molecule per cation–anion pair, which forms hydrogen bonds to one carbonyl group of the bpb ligand and to the terminal N atom of one cyanide ligand.

Related literature

The closely related neutral compound, $[Cr(bpb)(N_3)(H_2O)]\cdot H_2O$, has been reported previously (Ni *et al.*, 2006).



Experimental

Crystal data

$[Cr(CN)_2(C_{12}H_8N_2)_2][Cr(N_3)_2(C_{18}H_{12}N_4O_2)]\cdot H_2O$
M_r = 934.84
Monoclinic, $P2_1/c$
a = 12.3657 (5) Å
b = 20.8371 (10) Å
c = 15.9938 (5) Å
β = 105.48 (2)°
V = 3971.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 293 (2) K
0.43 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.778, T_{max} = 0.877
7868 measured reflections
6341 independent reflections
5953 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.164
S = 1.00
6341 reflections
592 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1W···N6^{i}	0.83 (3)	2.37 (4)	3.087 (6)	145 (2)
O3—H2W···O2	0.82 (4)	2.11 (3)	2.903 (5)	162 (3)

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

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: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2240).

References

Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Version 1.0-22. Bruker AXS Inc., Madison, Wisconsin, USA.
Ni, Z.-H., Kou, H.-Z., Zhang, L.-F., Ge, C., Wang, R.-J. & Cui, A.-L. (2006). *J. Chem. Crystallogr.* **36**, 465–472.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807049872

supplementary materials

Acta Cryst. (2007). E**63**, m2750 [**doi:10.1107/S1600536807049872**]

Bis(cyanido-κC)bis(1,10-phenanthroline-$\kappa^2 N,N'$)chromium(III) bis(azido-κN)[N,N'-(*o*-phenylene)bis(pyridine-2-carboxamide)-$\kappa^4 N$]chromate(III) monohydrate

G. Guan, Y. Gao, L. Wang and T. Wang

Comment

The title compound (Fig. 1) contains $[Cr^{III}(phen)_2(CN)_2]^+$ cations (phen = 1,10-phenanthroline) and $[Cr^{III}(bpb)(N_3)_2]^-$ anions (bpb = 1,2-bis(pyridine-2-carboxamido)benzene). In the cations, Cr^{III} is coordinated by two phen ligands and two cyanide ligands in a distorted octahderal geometry. In the anions, Cr^{III} is coordinated by the tetradentate bpb ligand and by two azide ions, also in a distorted octahedral geometry. There is one lattice water molecule per formula unit, which forms hydrogen bonds to one carboxyl group of the bpb ligand and to the terminal N atom of one azide ligand.

Experimental

A mixture of $K[Cr(bpb)(CN)_2]$ (0.1 mmol) (bpb = 1,2-bis(pyridine-2-carboxamido)benzene), $CrCl_3$ (0.1 mmol), phenthroline (0.2 mmol) and NaCN (0.5 mmol) in 20 ml e thanol (95%) was refluxed for two hours. The filtrate was evaporated under ambient conditions to give blue crystals with a yield of 26%. Elemental analysis calculated: 56.48, H 3.21, N 23.96%; found: C 56.41, H 3.26, N 23.89%.

Refinement

H atoms of the water molecule were located from difference Fourier maps and were refined with distance restraints of d(O—H) = 0.82 (2) Å and d(H···H) = 1.38 (2) Å. All other H atoms were placed in calculated positions with a C—H distance of 0.93%A and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

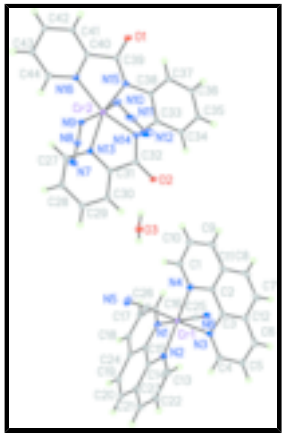


Fig. 1. The molecular structure of the title compound with displacement ellipsoids at 30% probability for non-H atoms.

Bis(cyanido-κ*C*)bis(1,10-phenanthroline-κ^2*N*,*N*')chromium(III) bis(azido-κ*N*)[*N*,*N*'-(*o*-phenylene)bis(pyridine-2-carboxamide)-\ κ^4*N*]chromate(III) monohydrate

Crystal data

$[Cr(CN)_2(C_{12}H_8N_2)_2][Cr(N_3)_2(C_{18}H_{12}N_4O_2)]\cdot H_2O$	F_{000} = 1912
M_r = 934.84	D_x = 1.564 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7263 reflections
a = 12.3657 (5) Å	θ = 3.1–25.4º
b = 20.8371 (10) Å	μ = 0.61 mm^{-1}
c = 15.9938 (5) Å	T = 293 (2) K
β = 105.48 (2)º	Block, blue
V = 3971.6 (3) Å^3	0.43 × 0.28 × 0.22 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	6341 independent reflections
Radiation source: fine-focus sealed tube	5953 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 293(2) K	θ_{max} = 25.4º
φ and ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = 0→14
T_{min} = 0.778, T_{max} = 0.877	k = 0→25
7868 measured reflections	l = −19→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.164	$w = 1/[\sigma^2(F_o^2) + (0.1141P)^2 + 0.9825P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
6341 reflections	$\Delta\rho_{max}$ = 1.13 e Å^{-3}
592 parameters	$\Delta\rho_{min}$ = −0.66 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Cr1	0.48484 (4)	0.43737 (2)	0.26437 (3)	0.02595 (15)
Cr2	0.04037 (4)	0.31652 (2)	0.78682 (3)	0.03055 (16)
C1	0.2625 (3)	0.42482 (19)	0.2972 (3)	0.0522 (9)
H1	0.2952	0.3995	0.3452	0.063*
C2	0.2781 (3)	0.48866 (17)	0.1825 (2)	0.0434 (8)
C3	0.3497 (3)	0.51591 (16)	0.1367 (2)	0.0404 (7)
C4	0.5315 (3)	0.52485 (16)	0.1276 (2)	0.0413 (7)
H4	0.6071	0.5144	0.1476	0.050*
C5	0.4983 (3)	0.56714 (17)	0.0582 (2)	0.0468 (8)
H5	0.5512	0.5844	0.0328	0.056*
C6	0.3861 (4)	0.58332 (18)	0.0271 (2)	0.0520 (9)
H6	0.3629	0.6115	−0.0193	0.062*
C7	0.1903 (4)	0.5694 (2)	0.0387 (3)	0.0621 (11)
H7	0.1607	0.5958	−0.0088	0.074*
C8	0.1225 (3)	0.5429 (2)	0.0821 (3)	0.0627 (12)
H8	0.0460	0.5517	0.0638	0.075*
C9	0.0973 (3)	0.4726 (2)	0.2051 (3)	0.0649 (12)
H9	0.0202	0.4794	0.1903	0.078*
C10	0.1471 (4)	0.4347 (2)	0.2746 (3)	0.0602 (11)
H10	0.1035	0.4154	0.3069	0.072*
C11	0.1633 (3)	0.5014 (2)	0.1560 (3)	0.0514 (9)
C12	0.3088 (3)	0.55702 (18)	0.0660 (2)	0.0476 (8)
C13	0.7315 (3)	0.45111 (17)	0.3061 (2)	0.0422 (8)
H13	0.7262	0.4862	0.3407	0.051*
C14	0.6471 (3)	0.36865 (15)	0.21236 (19)	0.0350 (7)
C15	0.5460 (3)	0.33696 (15)	0.1694 (2)	0.0364 (7)
C16	0.3544 (3)	0.33487 (18)	0.1428 (2)	0.0453 (8)
H16	0.2882	0.3517	0.1509	0.054*
C17	0.3481 (3)	0.28130 (19)	0.0884 (2)	0.0489 (9)
H17	0.2786	0.2635	0.0617	0.059*
C18	0.4425 (3)	0.25517 (17)	0.0742 (2)	0.0454 (8)
H18	0.4386	0.2196	0.0384	0.054*
C19	0.6524 (3)	0.26172 (16)	0.1054 (2)	0.0441 (8)

H19	0.6543	0.2265	0.0701	0.053*
C20	0.7495 (3)	0.29177 (17)	0.1467 (2)	0.0449 (8)
H20	0.8172	0.2770	0.1391	0.054*
C21	0.8467 (3)	0.37952 (18)	0.2482 (2)	0.0480 (9)
H21A	0.9169	0.3664	0.2441	0.058*
C22	0.8368 (3)	0.43136 (18)	0.2989 (3)	0.0496 (9)
H22A	0.9007	0.4535	0.3287	0.060*
C23	0.7489 (3)	0.34629 (16)	0.2024 (2)	0.0412 (8)
C24	0.5471 (3)	0.28382 (16)	0.1157 (2)	0.0389 (7)
C25	0.5217 (3)	0.50581 (17)	0.3445 (2)	0.0401 (7)
C26	0.5092 (4)	0.38279 (18)	0.3628 (3)	0.0527 (9)
C27	0.2940 (3)	0.27446 (17)	0.8456 (2)	0.0428 (8)
H27A	0.2757	0.2475	0.8861	0.051*
C28	0.4035 (3)	0.27802 (17)	0.8434 (2)	0.0443 (8)
H28A	0.4587	0.2546	0.8824	0.053*
C29	0.4307 (3)	0.31662 (17)	0.7827 (2)	0.0427 (8)
H29A	0.5047	0.3196	0.7799	0.051*
C30	0.3470 (3)	0.35126 (16)	0.7253 (2)	0.0375 (7)
H30A	0.3640	0.3773	0.6833	0.045*
C31	0.2383 (2)	0.34634 (14)	0.73160 (19)	0.0324 (6)
C32	0.1443 (3)	0.38415 (14)	0.67294 (19)	0.0324 (6)
C33	−0.0538 (2)	0.40797 (14)	0.65131 (19)	0.0308 (6)
C34	−0.0714 (3)	0.45215 (14)	0.58284 (19)	0.0336 (7)
H34A	−0.0111	0.4663	0.5633	0.040*
C35	−0.1787 (3)	0.47473 (15)	0.5442 (2)	0.0375 (7)
H35A	−0.1896	0.5042	0.4991	0.045*
C36	−0.2689 (3)	0.45414 (16)	0.5716 (2)	0.0401 (7)
H36A	−0.3405	0.4690	0.5440	0.048*
C37	−0.2541 (3)	0.41102 (15)	0.6405 (2)	0.0360 (7)
H37A	−0.3155	0.3974	0.6590	0.043*
C38	−0.1466 (2)	0.38841 (14)	0.68171 (18)	0.0311 (6)
C39	−0.1900 (3)	0.32288 (15)	0.7948 (2)	0.0363 (7)
C40	−0.1342 (3)	0.27376 (16)	0.8621 (2)	0.0369 (7)
C41	−0.1938 (3)	0.24040 (18)	0.9104 (2)	0.0456 (8)
H41A	−0.2692	0.2494	0.9042	0.055*
C42	−0.1398 (3)	0.19360 (18)	0.9678 (2)	0.0489 (9)
H42A	−0.1788	0.1707	1.0004	0.059*
C43	−0.0279 (3)	0.18105 (18)	0.9765 (2)	0.0478 (9)
H43A	0.0100	0.1497	1.0146	0.057*
C44	0.0258 (3)	0.21641 (18)	0.9268 (2)	0.0447 (8)
H44A	0.1013	0.2082	0.9323	0.054*
N1	0.4511 (2)	0.36252 (13)	0.18316 (18)	0.0399 (6)
N2	0.6385 (2)	0.41994 (13)	0.26382 (18)	0.0380 (6)
N3	0.4597 (2)	0.49880 (13)	0.16654 (17)	0.0379 (6)
N4	0.3275 (3)	0.45066 (14)	0.25173 (19)	0.0431 (7)
N5	0.5321 (3)	0.35103 (17)	0.4234 (2)	0.0685 (10)
N6	0.5450 (3)	0.54674 (15)	0.3951 (2)	0.0469 (7)
N7	0.0992 (4)	0.1976 (2)	0.6084 (3)	0.0872 (14)
N8	0.0586 (2)	0.21868 (15)	0.6591 (2)	0.0460 (7)

N9	0.0140 (2)	0.23669 (14)	0.71154 (19)	0.0426 (7)
N10	0.0900 (2)	0.38283 (15)	0.88229 (18)	0.0445 (7)
N11	0.1550 (3)	0.42486 (19)	0.8832 (2)	0.0622 (10)
N12	0.2133 (4)	0.4699 (3)	0.8812 (3)	0.1008 (17)
N13	0.2115 (2)	0.30835 (12)	0.79163 (17)	0.0342 (6)
N14	0.0490 (2)	0.37819 (12)	0.69435 (16)	0.0313 (5)
N15	−0.1182 (2)	0.34472 (12)	0.75171 (16)	0.0330 (6)
N16	−0.0246 (2)	0.26175 (13)	0.87136 (16)	0.0354 (6)
O1	−0.28966 (19)	0.33704 (12)	0.78477 (16)	0.0463 (6)
O2	0.16276 (18)	0.41634 (11)	0.61234 (14)	0.0378 (5)
O3	0.2764 (2)	0.36400 (13)	0.49047 (16)	0.0496 (6)
H1W	0.3414 (15)	0.377 (2)	0.511 (3)	0.074*
H2W	0.234 (3)	0.372 (2)	0.521 (2)	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0290 (3)	0.0261 (3)	0.0270 (3)	−0.00621 (17)	0.01505 (19)	−0.00410 (17)
Cr2	0.0273 (3)	0.0351 (3)	0.0315 (3)	−0.00147 (19)	0.0119 (2)	0.00456 (19)
C1	0.062 (2)	0.053 (2)	0.055 (2)	−0.0162 (18)	0.0374 (19)	−0.0139 (18)
C2	0.0443 (19)	0.0475 (19)	0.0448 (18)	−0.0044 (15)	0.0230 (15)	−0.0160 (16)
C3	0.0436 (18)	0.0435 (18)	0.0381 (17)	0.0036 (15)	0.0179 (14)	−0.0104 (14)
C4	0.0444 (19)	0.0417 (18)	0.0431 (18)	−0.0080 (15)	0.0209 (15)	−0.0045 (15)
C5	0.058 (2)	0.045 (2)	0.0438 (19)	−0.0030 (16)	0.0257 (17)	−0.0030 (16)
C6	0.074 (3)	0.047 (2)	0.0383 (18)	0.0046 (19)	0.0223 (18)	−0.0014 (16)
C7	0.059 (3)	0.074 (3)	0.052 (2)	0.020 (2)	0.0122 (19)	−0.010 (2)
C8	0.040 (2)	0.082 (3)	0.066 (3)	0.011 (2)	0.0132 (19)	−0.030 (2)
C9	0.043 (2)	0.078 (3)	0.080 (3)	−0.010 (2)	0.027 (2)	−0.038 (3)
C10	0.056 (2)	0.066 (3)	0.070 (3)	−0.020 (2)	0.037 (2)	−0.025 (2)
C11	0.042 (2)	0.063 (2)	0.054 (2)	0.0002 (17)	0.0214 (16)	−0.0219 (19)
C12	0.053 (2)	0.048 (2)	0.0437 (19)	0.0054 (16)	0.0161 (16)	−0.0095 (16)
C13	0.0380 (18)	0.0451 (19)	0.0433 (18)	−0.0026 (14)	0.0105 (14)	−0.0061 (15)
C14	0.0399 (17)	0.0323 (16)	0.0333 (15)	0.0013 (13)	0.0106 (13)	0.0021 (13)
C15	0.0415 (18)	0.0357 (16)	0.0337 (15)	−0.0013 (14)	0.0130 (13)	0.0027 (13)
C16	0.0381 (18)	0.055 (2)	0.0469 (19)	−0.0077 (16)	0.0177 (15)	−0.0042 (16)
C17	0.048 (2)	0.055 (2)	0.0469 (19)	−0.0154 (17)	0.0173 (16)	−0.0123 (17)
C18	0.059 (2)	0.0376 (18)	0.0415 (18)	−0.0088 (16)	0.0171 (16)	−0.0066 (14)
C19	0.050 (2)	0.0361 (17)	0.0451 (18)	0.0071 (15)	0.0099 (15)	−0.0039 (14)
C20	0.044 (2)	0.0423 (18)	0.0478 (19)	0.0142 (15)	0.0118 (15)	−0.0013 (15)
C21	0.0378 (19)	0.048 (2)	0.055 (2)	0.0061 (15)	0.0077 (16)	−0.0035 (17)
C22	0.0380 (19)	0.053 (2)	0.055 (2)	−0.0019 (16)	0.0068 (16)	−0.0107 (17)
C23	0.0392 (18)	0.0382 (18)	0.0434 (18)	0.0065 (14)	0.0063 (14)	0.0021 (14)
C24	0.049 (2)	0.0363 (17)	0.0322 (15)	−0.0022 (14)	0.0123 (14)	0.0007 (13)
C25	0.0387 (18)	0.0427 (19)	0.0433 (18)	−0.0027 (14)	0.0187 (14)	−0.0024 (15)
C26	0.070 (3)	0.046 (2)	0.050 (2)	−0.0174 (18)	0.0292 (19)	−0.0082 (18)
C27	0.0387 (18)	0.0460 (19)	0.0444 (18)	0.0002 (14)	0.0119 (14)	0.0072 (15)
C28	0.0372 (18)	0.0452 (19)	0.0478 (19)	0.0071 (15)	0.0067 (15)	0.0032 (15)
C29	0.0308 (17)	0.051 (2)	0.0467 (19)	−0.0015 (14)	0.0113 (14)	−0.0084 (15)

C30	0.0378 (17)	0.0387 (17)	0.0402 (17)	−0.0045 (14)	0.0178 (14)	−0.0026 (14)
C31	0.0301 (15)	0.0324 (16)	0.0364 (15)	−0.0045 (12)	0.0119 (12)	−0.0031 (13)
C32	0.0355 (16)	0.0316 (15)	0.0329 (15)	−0.0053 (12)	0.0142 (12)	−0.0018 (12)
C33	0.0325 (15)	0.0326 (15)	0.0293 (14)	−0.0001 (12)	0.0116 (12)	−0.0022 (12)
C34	0.0401 (17)	0.0314 (15)	0.0329 (15)	0.0017 (13)	0.0161 (13)	−0.0006 (12)
C35	0.0478 (19)	0.0348 (16)	0.0312 (15)	0.0054 (14)	0.0128 (13)	0.0036 (13)
C36	0.0411 (18)	0.0437 (18)	0.0358 (17)	0.0090 (14)	0.0109 (14)	0.0000 (14)
C37	0.0327 (16)	0.0402 (17)	0.0367 (16)	0.0019 (13)	0.0118 (13)	−0.0009 (13)
C38	0.0335 (16)	0.0346 (15)	0.0272 (14)	0.0015 (12)	0.0115 (12)	−0.0021 (12)
C39	0.0338 (17)	0.0415 (17)	0.0365 (16)	−0.0004 (13)	0.0144 (13)	0.0009 (13)
C40	0.0376 (17)	0.0419 (17)	0.0352 (16)	−0.0026 (14)	0.0167 (13)	0.0033 (14)
C41	0.0395 (19)	0.054 (2)	0.049 (2)	0.0008 (15)	0.0229 (15)	0.0087 (16)
C42	0.052 (2)	0.055 (2)	0.048 (2)	−0.0041 (17)	0.0267 (17)	0.0155 (17)
C43	0.051 (2)	0.051 (2)	0.0424 (19)	−0.0028 (16)	0.0138 (16)	0.0161 (16)
C44	0.0392 (18)	0.051 (2)	0.0444 (18)	0.0004 (15)	0.0125 (15)	0.0103 (16)
N1	0.0421 (15)	0.0381 (15)	0.0453 (15)	−0.0064 (12)	0.0220 (12)	−0.0026 (12)
N2	0.0404 (15)	0.0362 (14)	0.0386 (14)	−0.0024 (12)	0.0128 (12)	−0.0026 (11)
N3	0.0391 (15)	0.0396 (15)	0.0399 (14)	−0.0065 (12)	0.0187 (11)	−0.0074 (12)
N4	0.0469 (17)	0.0440 (16)	0.0440 (16)	−0.0104 (13)	0.0218 (13)	−0.0097 (13)
N5	0.095 (3)	0.055 (2)	0.054 (2)	−0.020 (2)	0.0180 (19)	0.0004 (17)
N6	0.0479 (18)	0.0486 (17)	0.0489 (17)	−0.0037 (14)	0.0211 (14)	−0.0035 (15)
N7	0.089 (3)	0.113 (4)	0.076 (3)	0.035 (3)	0.050 (2)	0.006 (2)
N8	0.0408 (16)	0.0495 (17)	0.0513 (17)	0.0063 (13)	0.0188 (14)	0.0057 (14)
N9	0.0369 (15)	0.0444 (16)	0.0546 (17)	−0.0076 (12)	0.0265 (13)	−0.0065 (13)
N10	0.0432 (16)	0.0536 (18)	0.0415 (15)	−0.0116 (14)	0.0194 (13)	−0.0065 (13)
N11	0.0462 (19)	0.079 (2)	0.071 (2)	−0.0131 (18)	0.0311 (17)	−0.0320 (19)
N12	0.093 (3)	0.113 (4)	0.121 (4)	−0.059 (3)	0.069 (3)	−0.061 (3)
N13	0.0320 (14)	0.0349 (14)	0.0364 (13)	−0.0023 (11)	0.0104 (11)	0.0027 (11)
N14	0.0288 (13)	0.0349 (13)	0.0328 (13)	−0.0004 (10)	0.0126 (10)	0.0004 (10)
N15	0.0315 (13)	0.0376 (14)	0.0331 (13)	0.0005 (11)	0.0140 (10)	0.0045 (11)
N16	0.0339 (14)	0.0404 (14)	0.0338 (13)	−0.0031 (11)	0.0120 (11)	0.0043 (11)
O1	0.0340 (13)	0.0608 (15)	0.0503 (14)	0.0072 (11)	0.0220 (10)	0.0127 (12)
O2	0.0386 (12)	0.0432 (12)	0.0371 (12)	−0.0007 (10)	0.0198 (10)	0.0076 (10)
O3	0.0512 (15)	0.0506 (15)	0.0526 (15)	0.0028 (12)	0.0233 (12)	−0.0019 (12)

Geometric parameters (Å, °)

Cr1—C25	1.890 (3)	C19—H19	0.930
Cr1—C26	1.899 (4)	C20—C23	1.445 (5)
Cr1—N4	1.922 (3)	C20—H20	0.930
Cr1—N2	1.936 (3)	C21—C22	1.375 (5)
Cr1—N3	1.981 (3)	C21—C23	1.416 (5)
Cr1—N1	2.001 (3)	C21—H21A	0.930
Cr2—N15	1.980 (3)	C22—H22A	0.930
Cr2—N14	1.984 (2)	C25—N6	1.158 (4)
Cr2—N9	2.028 (3)	C26—N5	1.145 (5)
Cr2—N10	2.029 (3)	C27—N13	1.348 (4)
Cr2—N16	2.087 (3)	C27—C28	1.366 (5)
Cr2—N13	2.104 (3)	C27—H27A	0.900

C1—N4	1.332 (5)	C28—C29	1.370 (5)
C1—C10	1.391 (6)	C28—H28A	0.930
C1—H1	0.930	C29—C30	1.388 (5)
C2—N4	1.365 (5)	C29—H29A	0.930
C2—C11	1.395 (5)	C30—C31	1.379 (4)
C2—C3	1.410 (5)	C30—H30A	0.930
C3—N3	1.362 (4)	C31—N13	1.352 (4)
C3—C12	1.401 (5)	C31—C32	1.506 (4)
C4—N3	1.329 (4)	C32—O2	1.249 (4)
C4—C5	1.391 (5)	C32—N14	1.318 (4)
C4—H4	0.930	C33—C34	1.402 (4)
C5—C6	1.384 (5)	C33—N14	1.417 (4)
C5—H5	0.930	C33—C38	1.420 (4)
C6—C12	1.385 (5)	C34—C35	1.387 (4)
C6—H6	0.930	C34—H34A	0.930
C7—C8	1.342 (7)	C35—C36	1.372 (5)
C7—C12	1.437 (6)	C35—H35A	0.930
C7—H7	0.930	C36—C37	1.396 (5)
C8—C11	1.444 (6)	C36—H36A	0.930
C8—H8	0.930	C37—C38	1.398 (4)
C9—C10	1.369 (7)	C37—H37A	0.930
C9—C11	1.407 (6)	C38—N15	1.413 (4)
C9—H9	0.930	C39—O1	1.235 (4)
C10—H10	0.930	C39—N15	1.340 (4)
C13—N2	1.337 (4)	C39—C40	1.512 (4)
C13—C22	1.399 (5)	C40—N16	1.347 (4)
C13—H13	0.930	C40—C41	1.388 (4)
C14—N2	1.370 (4)	C41—C42	1.383 (5)
C14—C23	1.391 (5)	C41—H41A	0.930
C14—C15	1.418 (4)	C42—C43	1.378 (5)
C15—N1	1.359 (4)	C42—H42A	0.930
C15—C24	1.403 (5)	C43—C44	1.378 (5)
C16—N1	1.330 (4)	C43—H43A	0.930
C16—C17	1.404 (5)	C44—N16	1.332 (4)
C16—H16	0.930	C44—H44A	0.930
C17—C18	1.361 (5)	N7—N8	1.149 (5)
C17—H17	0.930	N8—N9	1.180 (4)
C18—C24	1.419 (5)	N10—N11	1.187 (4)
C18—H18	0.930	N11—N12	1.189 (5)
C19—C20	1.360 (5)	O3—H1W	0.83 (3)
C19—C24	1.431 (5)	O3—H2W	0.82 (4)
C25—Cr1—C26	86.21 (15)	C21—C22—H22A	119.6
C25—Cr1—N4	90.95 (13)	C13—C22—H22A	119.6
C26—Cr1—N4	96.09 (16)	C14—C23—C21	116.8 (3)
C25—Cr1—N2	94.89 (13)	C14—C23—C20	119.2 (3)
C26—Cr1—N2	87.27 (15)	C21—C23—C20	124.0 (3)
N4—Cr1—N2	173.45 (12)	C15—C24—C18	117.5 (3)
C25—Cr1—N3	90.36 (13)	C15—C24—C19	118.8 (3)
C26—Cr1—N3	176.50 (13)	C18—C24—C19	123.7 (3)

N4—Cr1—N3	83.25 (12)	N6—C25—Cr1	178.4 (3)
N2—Cr1—N3	93.74 (11)	N5—C26—Cr1	175.0 (4)
C25—Cr1—N1	177.44 (13)	N13—C27—C28	122.8 (3)
C26—Cr1—N1	91.76 (14)	N13—C27—H27A	118.6
N4—Cr1—N1	90.82 (12)	C28—C27—H27A	118.6
N2—Cr1—N1	83.43 (11)	C27—C28—C29	118.8 (3)
N3—Cr1—N1	91.68 (11)	C27—C28—H28A	120.6
N15—Cr2—N14	80.93 (10)	C29—C28—H28A	120.6
N15—Cr2—N9	94.88 (11)	C28—C29—C30	119.6 (3)
N14—Cr2—N9	96.93 (11)	C28—C29—H29A	120.2
N15—Cr2—N10	95.10 (12)	C30—C29—H29A	120.2
N14—Cr2—N10	93.12 (11)	C31—C30—C29	118.8 (3)
N9—Cr2—N10	166.82 (13)	C31—C30—H30A	120.6
N15—Cr2—N16	79.77 (10)	C29—C30—H30A	120.6
N14—Cr2—N16	160.71 (10)	N13—C31—C30	121.6 (3)
N9—Cr2—N16	84.70 (11)	N13—C31—C32	117.0 (3)
N10—Cr2—N16	88.63 (11)	C30—C31—C32	121.4 (3)
N15—Cr2—N13	160.91 (10)	O2—C32—N14	127.8 (3)
N14—Cr2—N13	79.98 (10)	O2—C32—C31	119.6 (3)
N9—Cr2—N13	87.47 (10)	N14—C32—C31	112.5 (3)
N10—Cr2—N13	85.90 (11)	C34—C33—N14	126.8 (3)
N16—Cr2—N13	119.31 (10)	C34—C33—C38	119.0 (3)
N4—C1—C10	121.7 (4)	N14—C33—C38	114.2 (3)
N4—C1—H1	119.2	C35—C34—C33	120.1 (3)
C10—C1—H1	119.2	C35—C34—H34A	120.0
N4—C2—C11	123.7 (3)	C33—C34—H34A	120.0
N4—C2—C3	116.6 (3)	C36—C35—C34	120.9 (3)
C11—C2—C3	119.7 (3)	C36—C35—H35A	119.5
N3—C3—C12	123.7 (3)	C34—C35—H35A	119.5
N3—C3—C2	114.8 (3)	C35—C36—C37	120.4 (3)
C12—C3—C2	121.6 (3)	C35—C36—H36A	119.8
N3—C4—C5	122.7 (3)	C37—C36—H36A	119.8
N3—C4—H4	118.6	C36—C37—C38	119.8 (3)
C5—C4—H4	118.6	C36—C37—H37A	120.1
C6—C5—C4	119.7 (3)	C38—C37—H37A	120.1
C6—C5—H5	120.2	C37—C38—N15	126.5 (3)
C4—C5—H5	120.2	C37—C38—C33	119.7 (3)
C12—C6—C5	119.2 (4)	N15—C38—C33	113.8 (3)
C12—C6—H6	120.4	O1—C39—N15	128.8 (3)
C5—C6—H6	120.4	O1—C39—C40	120.3 (3)
C8—C7—C12	119.8 (4)	N15—C39—C40	110.9 (3)
C8—C7—H7	120.1	N16—C40—C41	120.9 (3)
C12—C7—H7	120.1	N16—C40—C39	117.3 (3)
C7—C8—C11	122.7 (4)	C41—C40—C39	121.8 (3)
C7—C8—H8	118.6	C42—C41—C40	119.3 (3)
C11—C8—H8	118.6	C42—C41—H41A	120.4
C10—C9—C11	119.8 (4)	C40—C41—H41A	120.4
C10—C9—H9	120.1	C43—C42—C41	119.6 (3)
C11—C9—H9	120.1	C43—C42—H42A	120.2

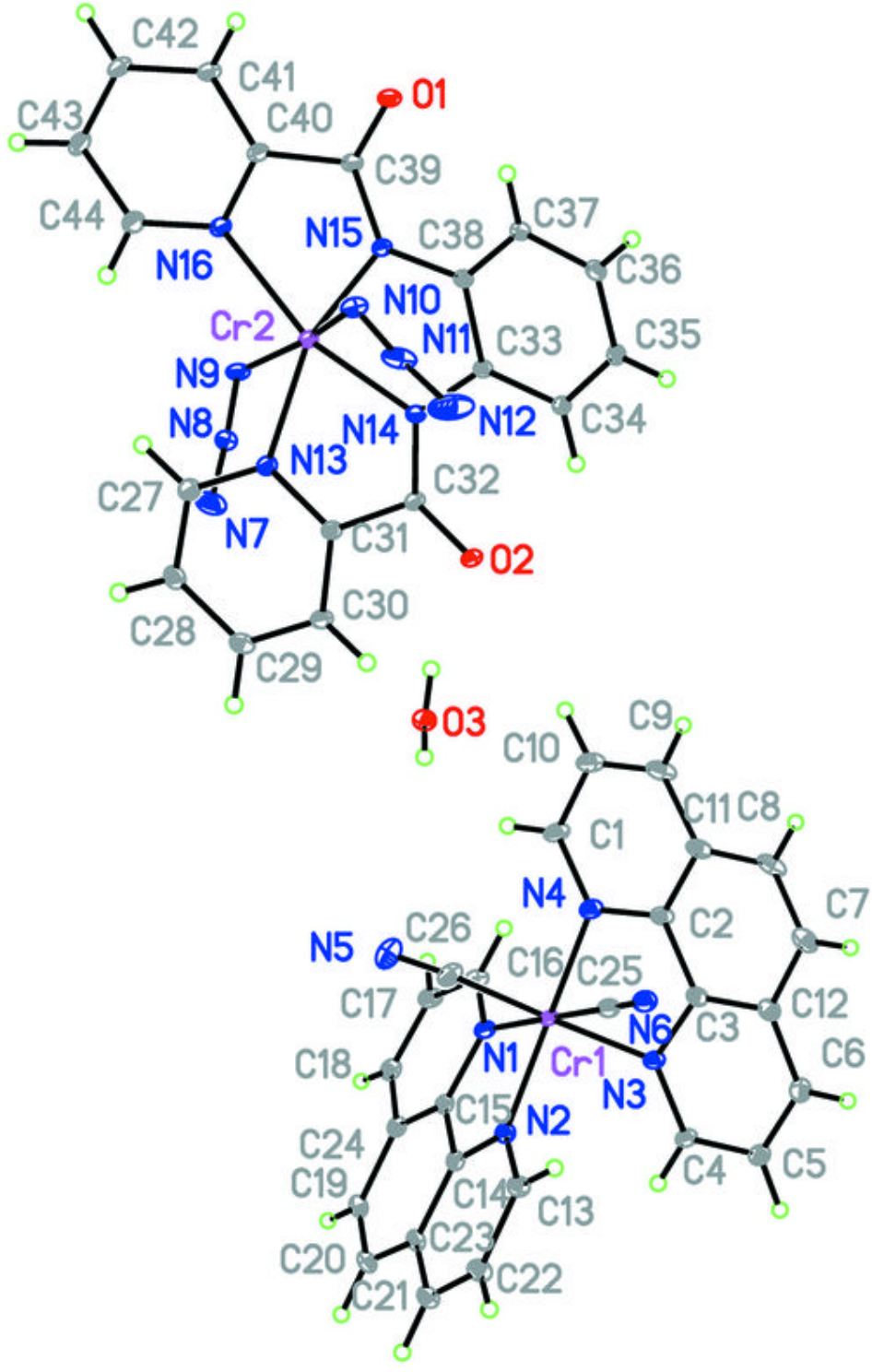
C9—C10—C1	120.2 (4)	C41—C42—H42A	120.2
C9—C10—H10	119.9	C42—C43—C44	117.8 (3)
C1—C10—H10	119.9	C42—C43—H43A	121.1
C2—C11—C9	116.4 (4)	C44—C43—H43A	121.1
C2—C11—C8	117.9 (4)	N16—C44—C43	123.4 (3)
C9—C11—C8	125.7 (4)	N16—C44—H44A	118.3
C6—C12—C3	117.4 (3)	C43—C44—H44A	118.3
C6—C12—C7	124.2 (4)	C16—N1—C15	117.1 (3)
C3—C12—C7	118.3 (4)	C16—N1—Cr1	131.1 (2)
N2—C13—C22	120.6 (3)	C15—N1—Cr1	111.8 (2)
N2—C13—H13	119.7	C13—N2—C14	119.2 (3)
C22—C13—H13	119.7	C13—N2—Cr1	128.3 (2)
N2—C14—C23	123.2 (3)	C14—N2—Cr1	112.5 (2)
N2—C14—C15	117.0 (3)	C4—N3—C3	117.3 (3)
C23—C14—C15	119.7 (3)	C4—N3—Cr1	130.6 (2)
N1—C15—C24	123.9 (3)	C3—N3—Cr1	112.2 (2)
N1—C15—C14	115.2 (3)	C1—N4—C2	118.2 (3)
C24—C15—C14	120.9 (3)	C1—N4—Cr1	128.7 (3)
N1—C16—C17	122.6 (3)	C2—N4—Cr1	112.9 (2)
N1—C16—H16	118.7	N7—N8—N9	175.9 (4)
C17—C16—H16	118.7	N8—N9—Cr2	130.6 (2)
C18—C17—C16	120.9 (3)	N11—N10—Cr2	125.4 (2)
C18—C17—H17	119.6	N10—N11—N12	175.0 (5)
C16—C17—H17	119.6	C27—N13—C31	118.3 (3)
C17—C18—C24	118.0 (3)	C27—N13—Cr2	130.4 (2)
C17—C18—H18	121.0	C31—N13—Cr2	111.2 (2)
C24—C18—H18	121.0	C32—N14—C33	125.5 (3)
C20—C19—C24	120.6 (3)	C32—N14—Cr2	119.0 (2)
C20—C19—H19	119.7	C33—N14—Cr2	115.23 (19)
C24—C19—H19	119.7	C39—N15—C38	124.6 (3)
C19—C20—C23	120.8 (3)	C39—N15—Cr2	119.7 (2)
C19—C20—H20	119.6	C38—N15—Cr2	115.70 (19)
C23—C20—H20	119.6	C44—N16—C40	119.0 (3)
C22—C21—C23	119.4 (3)	C44—N16—Cr2	128.8 (2)
C22—C21—H21A	120.3	C40—N16—Cr2	112.1 (2)
C23—C21—H21A	120.3	H1W—O3—H2W	113 (3)
C21—C22—C13	120.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1W···N6^{i}	0.83 (3)	2.37 (4)	3.087 (6)	145 (2)
O3—H2W···O2	0.82 (4)	2.11 (3)	2.903 (5)	162 (3)

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

Fig. 1


C42
C41
O1
C43
C40
C39
C44
N15
C38
C37
N16
C36
N10
Cr2
N11
C33
C35
N9
N8
N14
N12
C34
N13
C32
C27
N7
C31
O2
C30
C28
C29
O3
C9
C10
C11
C8
C1
N4
C7
C26
C2
N5
C16
C25
C17
C12
N6
C3
C18
N1
Cr1
C6
N3
C15
N2
C24
C4
C5
C19
C14
C13
C23
C20
C22
C21