Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{2-[(pyridin-2-yl)methylideneamino]-benzoato-κ^3N,N',O}chromium(III) nitrate monohydrate

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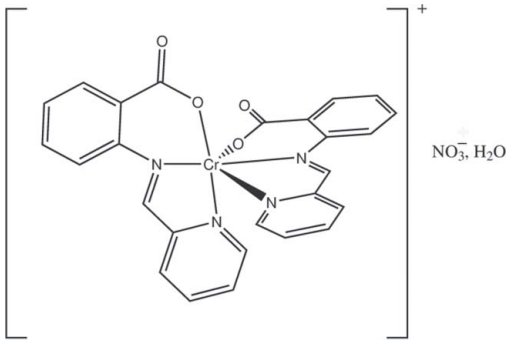
Received 11 March 2014; accepted 12 March 2014

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; H-atom completeness 91%; disorder in solvent or counterion; R factor = 0.057; wR factor = 0.136; data-to-parameter ratio = 11.2.

The title complex salt hydrate, $[Cr(C_{13}H_9N_2O_2)_2]NO_3\cdot H_2O$, comprises discrete cations, nitrate anions and solvent water molecules. The Cr^{III} atom is octahedrally coordinated by two anionic Schiff base ligands with the O atoms being *cis*. The two ligands differ significantly with dihedral angles between the pyridine and benzene rings of 4.8 (2) and 24.9 (2)°. The nitrate anion and solvent water molecule were modelled as being disordered, with the major components having site-occupancy values of 0.856 (14) and 0.727 (16), respectively. The crystal is built of alternating layers of cations and of anions plus water molecules, stacked along the *c* axis.

Related literature

For the synthesis of the Schiff base ligand and the structures of its complexes, see: Dey *et al.* (2003), Mukhopadhyay & Pal (2005); Sen *et al.* (2006).



Experimental

Crystal data

$[Cr(C_{13}H_9N_2O_2)_2]NO_3\cdot H_2O$
M_r = 582.47
Triclinic, $P\overline{1}$
a = 7.9131 (11) Å
b = 11.4929 (15) Å
c = 13.5627 (18) Å
α = 86.105 (11)°
β = 79.290 (11)°
γ = 85.566 (11)°
V = 1206.5 (3) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 4.47 mm^{-1}
T = 100 K
0.11 × 0.05 × 0.03 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.681, T_{max} = 0.892
9601 measured reflections
4251 independent reflections
2790 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.136
S = 0.99
4251 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cr1—O41	1.907 (3)	Cr1—N10	2.047 (3)
Cr1—O21	1.915 (3)	Cr1—N11	2.053 (3)
Cr1—N30	2.041 (3)	Cr1—N31	2.065 (3)

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

This work was partly supported by the State Fund for Fundamental Researches of Ukraine (project 54.3/005). The authors acknowledge the facilities, scientific and technical assistance of the Australian Microscopy & Microanalysis Research Facility at the Centre for Microscopy, Characterization & Analysis, the University of Western Australia, a facility funded by the University, and the State and Commonwealth Governments.

Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5300).

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supporting information

Acta Cryst. (2014). E**70**, m136 [doi:10.1107/S1600536814005649]

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S1. Structural commentary

The title compound was prepared during studies of the coordination behaviour of the tridentate carboxylate Schiff base ligand 2-*N*-(2′-pyridylimine)benzoic acid (HL) which results from the condensation between 2-pyridinecarbaldehide and anthranilic acid. Known metal complexes containing deprotonated HL (Dey *et al.*, 2003; Mukhopadhyay *et al.*, 2005; Sen *et al.*, 2006) were prepared by *in situ* Schiff base synthesis - a synthetic approach utilized in the present work as well.

The title compound, $Cr(C_{13}H_{10}N_2O_2)_2NO_3\cdot H_2O$, is formed of discrete $[CrL_2]^+$ cations, nitrate anions and solvent water molecules. The cation has no crystallographically imposed symmetry. The ligand molecules are deprotonated at the carboxylato oxygen atom and coordinate to the Cr^{III} atom through the azomethine, pyridine-N and carboxylato-O atoms in such a way that the metal atom is octahedrally surrounded by two anionic ligands with *cis* O atoms (Fig. 1 & Table 1). The Cr–N/O distances fall in the range 1.907 (3)–2.065 (3) Å, the *trans* angles at the metal atom lie in the range 170.57 (13)–173.61 (13), the *cis* angles vary from 80.47 (14) to 94.47 (14)°. The coordination geometry around the chromium centre is similar to that reported for $NiL_2\cdot H_2O$ (Mukhopadhyay *et al.*, 2005).

The two ligands differ significantly. The atoms of ligand 1 are virtually coplanar with the dihedral angle between the pyridyl and benzene rings being 4.8 (2)°. By contrast, in ligand 2 this dihedral angle is 24.9 (2)°.

The crystal lattice is built of alternating layers of cations and of anions plus water molecules (Fig. 2).

S2. Synthesis and crystallization

The ligand HL was prepared by refluxing 2-pyridinecarbaldehyde (0.38 ml, 4 mmol) with anthranilic acid (0.55 g, 4 mmol) in methanol (20 ml) for 0.5 h. The resultant yellow solution was left in open air overnight and used without further purification.

To a stirred methanol solution (10 ml) of $Cr(NO_3)_3\cdot 9H_2O$ (0.80 g, 2 mmol) in a 50 ml conic flask, HL in methanol from the previous preparation was added. The solution was magnetically stirred at 323 K for 20 minutes. The brown precipitate was filtered off. The red-brown solution was left to evaporate at room temperature. Red-brown rod-like microcrystals of the title compound were formed in a few days. They were collected by filter-suction, washed with dry Pr^iOH and finally dried *in vacuo* (yield: 45%).

S3. Refinement

The nitrate anion and solvent water molecule were modelled as being disordered. The site occupancy factors of the major component of the nitrate refined to 0.856 (14), and that of the disordered water molecule to 0.727 (16). Minor components of the disordered atoms were refined with isotropic displacement parameters. Water molecule hydrogen atoms were not located. All remaining hydrogen atoms were added at calculated positions (C—H = 0.95 Å) and refined by use of a riding model, with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

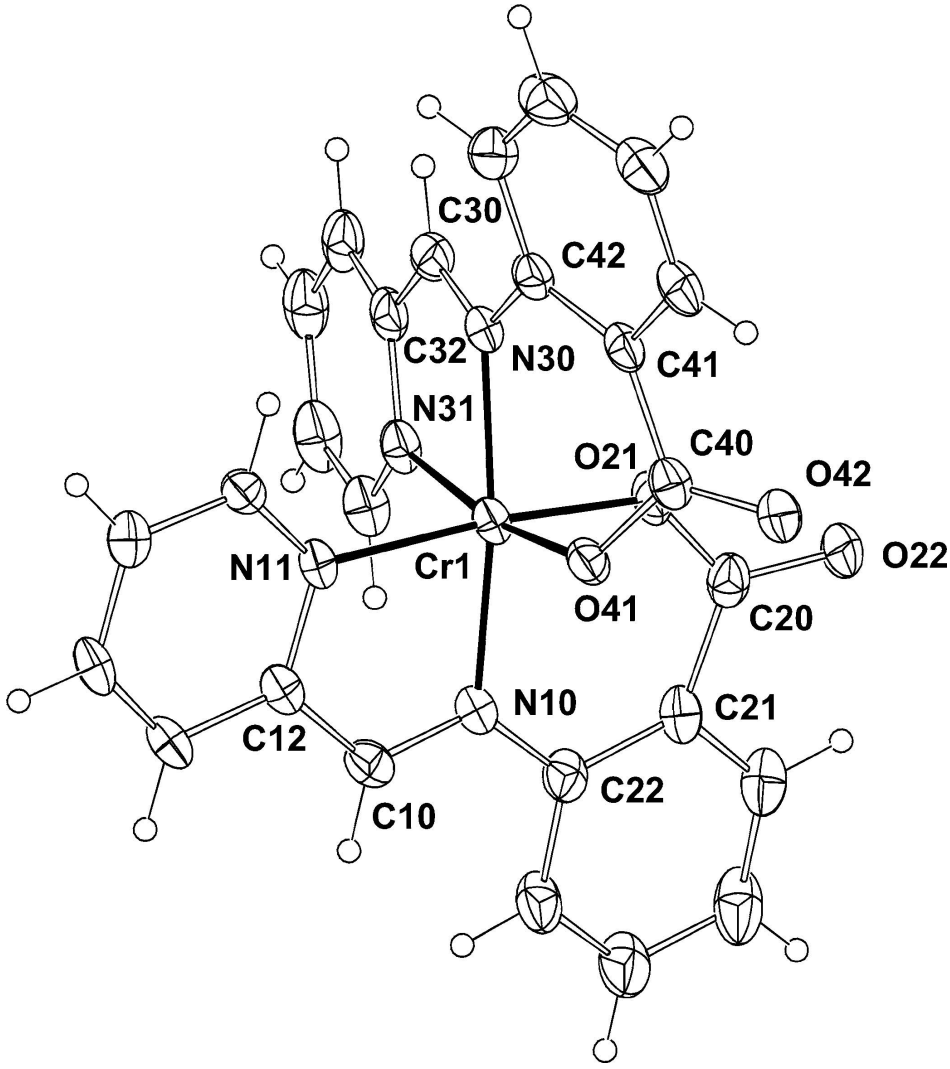

Figure 1

Molecular structure of the cation with the numbering scheme (the non-hydrogen atoms shown as 50% atomic displacement ellipsoids).

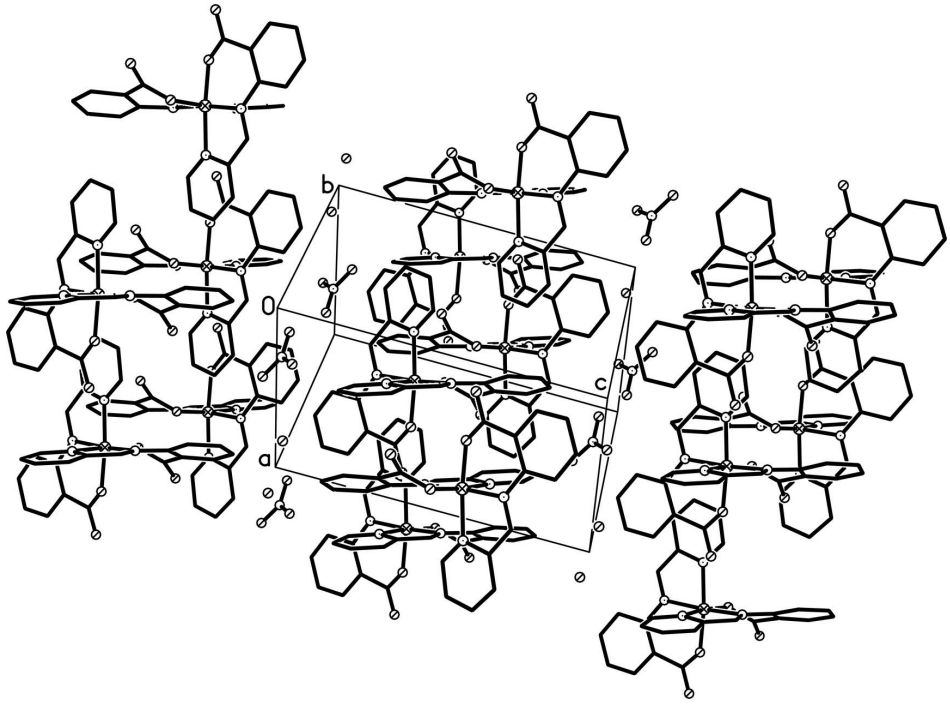

Figure 2

Packing diagram showing alternating layers of $[CrL_2]^+$ cations and nitrate anions plus solvent water molecules (C-bound H atoms and minor components of the disordered nitrate and water molecules are omitted for clarity).

Bis{2-[(pyridin-2-yl)methylideneamino]benzoato-κ^3N,N',O}chromium(III) nitrate monohydrate

Crystal data

$[Cr(C_{13}H_9N_2O_2)_2]NO_3 \cdot H_2O$
$M_r = 582.47$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.9131$ (11) Å
$b = 11.4929$ (15) Å
$c = 13.5627$ (18) Å
$\alpha = 86.105$ (11)°
$\beta = 79.290$ (11)°
$\gamma = 85.566$ (11)°
$V = 1206.5$ (3) Å^3
$Z = 2$
$F(000) = 598$
$D_x = 1.603$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 1206 reflections
$\theta = 3.3$–$67.2°$
$\mu = 4.47$ mm^{-1}
$T = 100$ K
Rod, red-brown
0.11 × 0.05 × 0.03 mm

Data collection

Oxford Diffraction Gemini diffractometer
Graphite monochromator
Detector resolution: 10.4738 pixels mm^{-1}
ω scans
Absorption correction: analytical (Clark & Reid, 1995)
$T_{min} = 0.681$, $T_{max} = 0.892$
9601 measured reflections
4251 independent reflections
2790 reflections with $I > 2\sigma(I)$
$R_{int} = 0.083$
$\theta_{max} = 67.0°$, $\theta_{min} = 3.3°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 13$
$l = -10 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.136$
$S = 0.99$
4251 reflections
379 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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. The nitrate anion and solvent water molecule were modelled as being disordered. The site occupancy factors of the two components of the nitrate refined to 0.856 (14) and its complement. Those for the two components of the disordered water molecule appeared to be significantly different and were refined to 0.727 (16) and its complement. Minor components of the disordered atoms were refined with isotropic displacement parameters. Water molecule hydrogen atoms were not located.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cr1	0.54166 (9)	0.74547 (6)	0.61375 (5)	0.0373 (2)	
N11	0.7561 (4)	0.6436 (3)	0.6386 (2)	0.0358 (8)	
C12	0.7217 (6)	0.5754 (4)	0.7256 (3)	0.0413 (10)	
C13	0.8463 (6)	0.4967 (4)	0.7569 (3)	0.0477 (11)	
H13	0.821	0.4509	0.8182	0.057*	
C14	1.0056 (6)	0.4866 (4)	0.6976 (3)	0.0491 (11)	
H14	1.0916	0.4319	0.7167	0.059*	
C15	1.0425 (6)	0.5553 (4)	0.6101 (3)	0.0452 (10)	
H15	1.1539	0.5499	0.5692	0.054*	
C16	0.9120 (5)	0.6332 (4)	0.5828 (3)	0.0382 (9)	
H16	0.9362	0.6803	0.5222	0.046*	
C10	0.5485 (6)	0.5899 (4)	0.7818 (3)	0.0437 (10)	
H10	0.5167	0.5473	0.8442	0.052*	
N10	0.4359 (4)	0.6618 (3)	0.7463 (2)	0.0385 (8)	
C21	0.1464 (6)	0.7587 (4)	0.7554 (3)	0.0445 (10)	
C22	0.2644 (6)	0.6824 (4)	0.7983 (3)	0.0442 (10)	
C23	0.2101 (6)	0.6264 (5)	0.8926 (3)	0.0585 (13)	
H23	0.2878	0.5734	0.9215	0.07*	
C24	0.0447 (7)	0.6481 (6)	0.9433 (3)	0.0738 (17)	
H24	0.0101	0.6101	1.0075	0.089*	
C25	−0.0730 (7)	0.7238 (6)	0.9031 (4)	0.0772 (19)	

H25	−0.1872	0.7381	0.9387	0.093*	
C26	−0.0193 (6)	0.7777 (5)	0.8101 (4)	0.0597 (13)	
H26	−0.0987	0.8301	0.782	0.072*	
C20	0.1775 (6)	0.8256 (4)	0.6544 (3)	0.0457 (10)	
O21	0.3303 (4)	0.8357 (3)	0.6057 (2)	0.0465 (7)	
O22	0.0532 (4)	0.8712 (3)	0.6203 (3)	0.0635 (9)	
N31	0.6119 (5)	0.8854 (3)	0.6813 (2)	0.0418 (8)	
C32	0.6966 (6)	0.9635 (4)	0.6123 (3)	0.0467 (11)	
C33	0.7415 (6)	1.0696 (4)	0.6378 (4)	0.0548 (12)	
H33	0.7988	1.1224	0.588	0.066*	
C34	0.7011 (7)	1.0973 (4)	0.7376 (4)	0.0619 (14)	
H34	0.732	1.1692	0.7576	0.074*	
C35	0.6163 (7)	1.0201 (5)	0.8070 (4)	0.0620 (14)	
H35	0.5875	1.0384	0.8756	0.074*	
C36	0.5720 (6)	0.9140 (4)	0.7769 (3)	0.0538 (12)	
H36	0.5123	0.8612	0.8257	0.065*	
C30	0.7297 (6)	0.9282 (4)	0.5101 (3)	0.0449 (10)	
H30	0.7933	0.9752	0.4581	0.054*	
N30	0.6723 (4)	0.8323 (3)	0.4901 (2)	0.0397 (8)	
C41	0.5867 (5)	0.7161 (4)	0.3666 (3)	0.0399 (10)	
C42	0.6963 (5)	0.7961 (4)	0.3896 (3)	0.0419 (10)	
C43	0.8237 (6)	0.8424 (4)	0.3149 (3)	0.0547 (12)	
H43	0.9	0.8948	0.3316	0.066*	
C44	0.8384 (7)	0.8117 (5)	0.2164 (3)	0.0623 (14)	
H44	0.9261	0.842	0.1658	0.075*	
C45	0.7261 (7)	0.7375 (5)	0.1919 (3)	0.0571 (13)	
H45	0.7342	0.7187	0.124	0.069*	
C46	0.6018 (6)	0.6903 (4)	0.2656 (3)	0.0485 (11)	
H46	0.525	0.6393	0.2476	0.058*	
C40	0.4502 (6)	0.6555 (4)	0.4412 (3)	0.0415 (10)	
O41	0.4786 (4)	0.6332 (2)	0.53221 (18)	0.0402 (7)	
O42	0.3241 (4)	0.6254 (3)	0.4119 (2)	0.0503 (8)	
N1	0.4349 (7)	0.7154 (5)	1.0410 (3)	0.0656 (12)	
O11	0.5173 (8)	0.6206 (5)	1.0362 (4)	0.078 (2)	0.856 (14)
O12	0.2875 (9)	0.7275 (7)	1.0988 (3)	0.078 (2)	0.856 (14)
O13	0.4921 (9)	0.8027 (4)	0.9909 (3)	0.0713 (17)	0.856 (14)
O14	0.354 (3)	0.668 (2)	1.1045 (15)	0.031 (7)*	0.144 (14)
O15	0.561 (5)	0.656 (4)	0.982 (3)	0.089 (12)*	0.144 (14)
O16	0.389 (7)	0.816 (4)	0.995 (3)	0.092 (12)*	0.144 (14)
O1	0.1743 (16)	0.9903 (10)	0.9800 (8)	0.185 (6)	0.727 (16)
O2	0.129 (2)	0.9116 (18)	1.0468 (15)	0.100 (8)*	0.273 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0381 (4)	0.0373 (4)	0.0385 (3)	0.0040 (3)	−0.0158 (3)	0.0012 (3)
N11	0.037 (2)	0.0369 (19)	0.0365 (16)	0.0042 (15)	−0.0163 (15)	−0.0046 (14)
C12	0.046 (3)	0.040 (2)	0.040 (2)	0.003 (2)	−0.0167 (19)	−0.0007 (18)

C13	0.055 (3)	0.047 (3)	0.043 (2)	0.010 (2)	−0.021 (2)	0.0056 (19)
C14	0.048 (3)	0.049 (3)	0.052 (2)	0.016 (2)	−0.025 (2)	0.000 (2)
C15	0.040 (2)	0.048 (3)	0.050 (2)	0.005 (2)	−0.0144 (19)	−0.011 (2)
C16	0.044 (3)	0.036 (2)	0.0366 (19)	−0.0026 (18)	−0.0126 (18)	0.0002 (17)
C10	0.054 (3)	0.043 (2)	0.0354 (19)	−0.002 (2)	−0.0125 (19)	0.0000 (18)
N10	0.040 (2)	0.040 (2)	0.0370 (16)	0.0031 (16)	−0.0134 (15)	−0.0011 (15)
C21	0.041 (2)	0.049 (3)	0.047 (2)	0.005 (2)	−0.0178 (19)	−0.013 (2)
C22	0.045 (3)	0.056 (3)	0.034 (2)	−0.005 (2)	−0.0132 (18)	−0.0095 (19)
C23	0.047 (3)	0.091 (4)	0.039 (2)	0.004 (3)	−0.015 (2)	−0.004 (2)
C24	0.052 (3)	0.133 (6)	0.036 (2)	−0.003 (3)	−0.008 (2)	0.003 (3)
C25	0.045 (3)	0.136 (6)	0.050 (3)	0.012 (3)	−0.011 (2)	−0.024 (3)
C26	0.045 (3)	0.078 (4)	0.061 (3)	0.003 (3)	−0.020 (2)	−0.019 (3)
C20	0.041 (3)	0.034 (2)	0.067 (3)	−0.0011 (19)	−0.022 (2)	−0.006 (2)
O21	0.0393 (18)	0.0467 (18)	0.0559 (16)	0.0077 (14)	−0.0209 (14)	0.0026 (14)
O22	0.0394 (18)	0.057 (2)	0.094 (2)	0.0046 (16)	−0.0276 (17)	0.0244 (18)
N31	0.043 (2)	0.0366 (19)	0.0499 (19)	0.0056 (16)	−0.0218 (16)	−0.0053 (16)
C32	0.040 (2)	0.036 (2)	0.069 (3)	0.006 (2)	−0.028 (2)	0.003 (2)
C33	0.045 (3)	0.036 (3)	0.090 (3)	0.007 (2)	−0.033 (2)	−0.006 (2)
C34	0.059 (3)	0.041 (3)	0.096 (4)	0.013 (2)	−0.042 (3)	−0.018 (3)
C35	0.066 (3)	0.055 (3)	0.075 (3)	0.016 (3)	−0.037 (3)	−0.022 (3)
C36	0.053 (3)	0.055 (3)	0.058 (3)	0.008 (2)	−0.023 (2)	−0.007 (2)
C30	0.040 (2)	0.036 (2)	0.060 (3)	0.0017 (19)	−0.017 (2)	0.006 (2)
N30	0.0346 (19)	0.041 (2)	0.0443 (18)	0.0032 (16)	−0.0158 (15)	0.0069 (15)
C41	0.036 (2)	0.045 (2)	0.038 (2)	0.0094 (19)	−0.0125 (17)	0.0020 (18)
C42	0.035 (2)	0.044 (2)	0.045 (2)	0.0065 (19)	−0.0117 (18)	0.0069 (18)
C43	0.043 (3)	0.058 (3)	0.060 (3)	0.002 (2)	−0.008 (2)	0.007 (2)
C44	0.053 (3)	0.074 (4)	0.051 (3)	0.010 (3)	0.003 (2)	0.012 (2)
C45	0.054 (3)	0.070 (3)	0.043 (2)	0.016 (3)	−0.008 (2)	0.005 (2)
C46	0.049 (3)	0.049 (3)	0.046 (2)	0.019 (2)	−0.016 (2)	−0.001 (2)
C40	0.043 (3)	0.038 (2)	0.045 (2)	0.0071 (19)	−0.0155 (19)	−0.0049 (18)
O41	0.0452 (17)	0.0414 (16)	0.0371 (13)	−0.0019 (13)	−0.0171 (12)	0.0030 (11)
O42	0.0506 (19)	0.060 (2)	0.0462 (15)	−0.0083 (15)	−0.0226 (14)	0.0020 (14)
N1	0.085 (4)	0.070 (3)	0.047 (2)	−0.014 (3)	−0.024 (2)	0.006 (2)
O11	0.115 (4)	0.058 (3)	0.068 (4)	0.007 (3)	−0.040 (3)	0.002 (3)
O12	0.081 (4)	0.099 (5)	0.051 (2)	−0.014 (4)	0.001 (2)	−0.014 (3)
O13	0.067 (4)	0.077 (3)	0.063 (3)	0.005 (3)	−0.008 (2)	0.024 (2)
O1	0.227 (12)	0.165 (10)	0.144 (8)	0.048 (9)	−0.028 (8)	0.044 (7)

Geometric parameters (Å, º)

Cr1—O41	1.907 (3)	N31—C36	1.334 (6)
Cr1—O21	1.915 (3)	N31—C32	1.369 (6)
Cr1—N30	2.041 (3)	C32—C33	1.380 (6)
Cr1—N10	2.047 (3)	C32—C30	1.442 (6)
Cr1—N11	2.053 (3)	C33—C34	1.385 (7)
Cr1—N31	2.065 (3)	C33—H33	0.95
N11—C16	1.323 (5)	C34—C35	1.367 (8)
N11—C12	1.367 (5)	C34—H34	0.95

C12—C13	1.391 (6)	C35—C36	1.401 (7)
C12—C10	1.443 (6)	C35—H35	0.95
C13—C14	1.365 (7)	C36—H36	0.95
C13—H13	0.95	C30—N30	1.287 (5)
C14—C15	1.377 (6)	C30—H30	0.95
C14—H14	0.95	N30—C42	1.427 (5)
C15—C16	1.400 (6)	C41—C42	1.400 (6)
C15—H15	0.95	C41—C46	1.403 (6)
C16—H16	0.95	C41—C40	1.513 (6)
C10—N10	1.304 (5)	C42—C43	1.398 (6)
C10—H10	0.95	C43—C44	1.387 (7)
N10—C22	1.418 (6)	C43—H43	0.95
C21—C26	1.390 (7)	C44—C45	1.375 (8)
C21—C22	1.409 (6)	C44—H44	0.95
C21—C20	1.513 (7)	C45—C46	1.380 (7)
C22—C23	1.401 (6)	C45—H45	0.95
C23—C24	1.373 (7)	C46—H46	0.95
C23—H23	0.95	C40—O42	1.222 (5)
C24—C25	1.386 (8)	C40—O41	1.300 (5)
C24—H24	0.95	N1—O14	1.11 (2)
C25—C26	1.375 (8)	N1—O11	1.225 (7)
C25—H25	0.95	N1—O13	1.239 (7)
C26—H26	0.95	N1—O12	1.282 (8)
C20—O22	1.229 (5)	N1—O15	1.33 (4)
C20—O21	1.275 (5)	N1—O16	1.33 (4)

O41—Cr1—O21	89.52 (12)	O22—C20—O21	120.4 (4)
O41—Cr1—N30	91.12 (13)	O22—C20—C21	119.0 (4)
O21—Cr1—N30	92.67 (13)	O21—C20—C21	120.6 (4)
O41—Cr1—N10	94.27 (13)	C20—O21—Cr1	131.4 (3)
O21—Cr1—N10	92.10 (14)	C36—N31—C32	118.1 (4)
N30—Cr1—N10	172.82 (14)	C36—N31—Cr1	129.7 (3)
O41—Cr1—N11	92.27 (12)	C32—N31—Cr1	111.8 (3)
O21—Cr1—N11	173.61 (13)	N31—C32—C33	122.8 (4)
N30—Cr1—N11	93.43 (14)	N31—C32—C30	114.8 (4)
N10—Cr1—N11	81.65 (14)	C33—C32—C30	122.4 (5)
O41—Cr1—N31	170.57 (13)	C32—C33—C34	118.4 (5)
O21—Cr1—N31	86.65 (13)	C32—C33—H33	120.8
N30—Cr1—N31	80.47 (14)	C34—C33—H33	120.8
N10—Cr1—N31	94.47 (14)	C35—C34—C33	119.3 (5)
N11—Cr1—N31	92.48 (13)	C35—C34—H34	120.3
C16—N11—C12	118.7 (3)	C33—C34—H34	120.3
C16—N11—Cr1	130.0 (3)	C34—C35—C36	120.0 (5)
C12—N11—Cr1	111.3 (3)	C34—C35—H35	120
N11—C12—C13	121.7 (4)	C36—C35—H35	120
N11—C12—C10	115.7 (4)	N31—C36—C35	121.4 (5)
C13—C12—C10	122.6 (4)	N31—C36—H36	119.3
C14—C13—C12	118.5 (4)	C35—C36—H36	119.3

C14—C13—H13	120.7	N30—C30—C32	119.4 (4)
C12—C13—H13	120.7	N30—C30—H30	120.3
C13—C14—C15	120.4 (4)	C32—C30—H30	120.3
C13—C14—H14	119.8	C30—N30—C42	121.3 (4)
C15—C14—H14	119.8	C30—N30—Cr1	113.3 (3)
C14—C15—C16	118.4 (4)	C42—N30—Cr1	125.3 (3)
C14—C15—H15	120.8	C42—C41—C46	117.7 (4)
C16—C15—H15	120.8	C42—C41—C40	125.8 (3)
N11—C16—C15	122.3 (4)	C46—C41—C40	116.5 (4)
N11—C16—H16	118.9	C43—C42—C41	120.7 (4)
C15—C16—H16	118.9	C43—C42—N30	120.6 (4)
N10—C10—C12	119.5 (4)	C41—C42—N30	118.7 (4)
N10—C10—H10	120.2	C44—C43—C42	119.8 (5)
C12—C10—H10	120.2	C44—C43—H43	120.1
C10—N10—C22	122.7 (4)	C42—C43—H43	120.1
C10—N10—Cr1	111.8 (3)	C45—C44—C43	120.1 (5)
C22—N10—Cr1	125.4 (3)	C45—C44—H44	119.9
C26—C21—C22	118.3 (4)	C43—C44—H44	119.9
C26—C21—C20	114.1 (4)	C44—C45—C46	120.3 (4)
C22—C21—C20	127.6 (4)	C44—C45—H45	119.9
C23—C22—C21	119.2 (4)	C46—C45—H45	119.9
C23—C22—N10	120.3 (4)	C45—C46—C41	121.3 (5)
C21—C22—N10	120.5 (4)	C45—C46—H46	119.4
C24—C23—C22	120.1 (5)	C41—C46—H46	119.4
C24—C23—H23	120	O42—C40—O41	123.6 (4)
C22—C23—H23	120	O42—C40—C41	118.6 (4)
C23—C24—C25	121.7 (5)	O41—C40—C41	117.6 (4)
C23—C24—H24	119.2	C40—O41—Cr1	124.6 (3)
C25—C24—H24	119.2	O11—N1—O13	121.1 (6)
C26—C25—C24	117.9 (5)	O11—N1—O12	120.9 (6)
C26—C25—H25	121	O13—N1—O12	118.0 (6)
C24—C25—H25	121	O14—N1—O15	119 (2)
C25—C26—C21	122.7 (5)	O14—N1—O16	126 (2)
C25—C26—H26	118.6	O15—N1—O16	111 (2)
C21—C26—H26	118.6		