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Sodium *cis*-bis(iminodiacetato-κ^3N,O,O')-chromate(III) sesquihydrate

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In the title compound, $Na[Cr(C_4H_5NO_4)_2]\cdot1.5H_2O$, the Cr^{III}-centered complex anion displays an octahedral coordination geometry formed by two facial iminodiacetate dianions, with two N atoms in a *cis* configuration. The Na^+ ion is surrounded by one water and five carboxyl O atoms, with Na—O distances of 2.3221 (15)-2.5531 (18) Å. There is an extensive hydrogen-bonding network in the crystal structure.

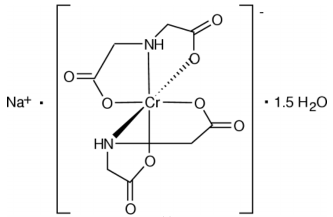
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.075
Data-to-parameter ratio = 15.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The iminodiacetate dianion (IDA) and its alkyl-substituted derivatives with an alkyl substituent on the N atom form several stable 2:1 metal complexes, in which each tridentate IDA ligand forms two five-membered chelate rings with the central metal ion (Nesterova *et al.*, 1979; Mootz & Wunderlich, 1980; Suh *et al.*, 1997). The title compound, (I), has been obtained recently in this laboratory.



(I)

The asymmetric unit of (I) consists of two Cr^{III} complex anions, two Na^+ ions and three water molecules (Fig. 1). The Cr^{III}-centered complex anions display an approximately octahedral coordination. Two IDA ligands facially chelate to each Cr atom, with two N atoms in a *cis* configuration. The *cis* geometry was also reported for potassium bis(iminodiacetato)chromate (Mootz & Wunderlich, 1980), although a *trans* configuration was observed in sodium bis(iminodiacetato)cobaltate (Nesterova *et al.*, 1979) and in sodium bis(methyliminodiacetato)chromate (Suh *et al.*, 1997). The two IDA ligands in each complex anion form four five-membered chelate rings with the Cr atom. Two rings show envelope conformations, with the N atoms at the flap positions displaced out of the mean planes of other four atoms by 0.3784 (14) (O11-ring) and 0.5305 (15) Å (O17-ring) in the Cr1 complex, and by 0.5255 (16) (O21-ring) and 0.4588 (16) Å (O27-ring) in the Cr2 complex. The other two chelate rings in both Cr1 and Cr2 complexes are planar, the maximum atomic deviation being 0.0817 (18) Å (C13).

Each Na^+ atom is surrounded by one water and five carboxyl O atoms, in a distorted octahedral coordination. The Na1—O and Na2—O distances are 2.3427 (16)–2.4179 (15)

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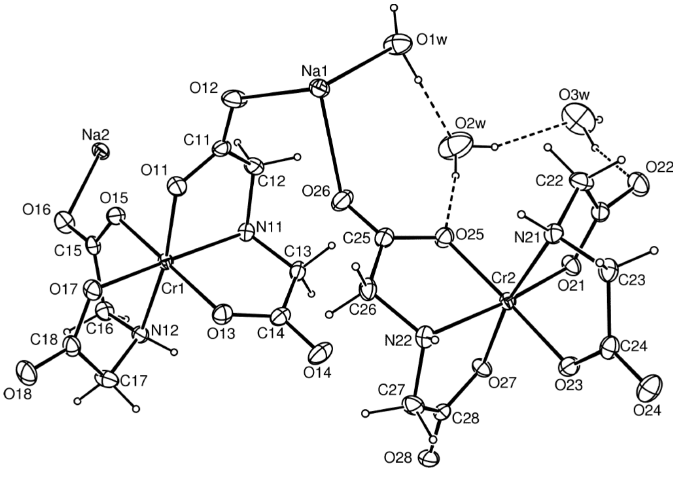

Figure 1

The structure of the asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level. Dashed lines indicate hydrogen bonds.

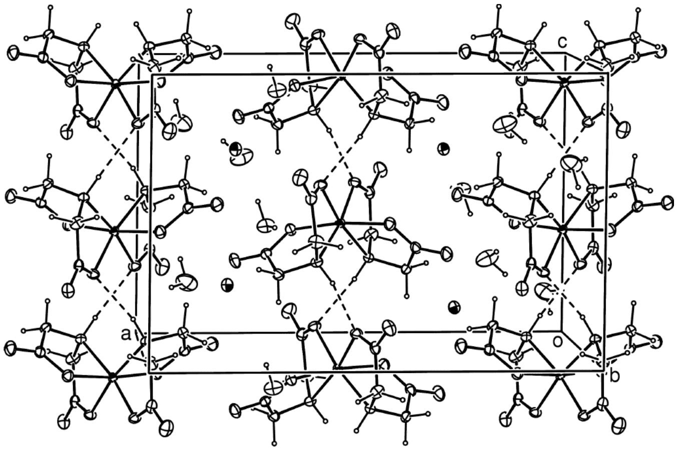

Figure 2

A packing diagram of (I). Dashed lines indicate hydrogen bonds between Cr^{III} complex anions. The coordination bonds for Na^+ atoms and hydrogen bonds involving water molecules have been omitted for clarity.

and 2.3221 (15)–2.5531 (18) Å, respectively (Table 1). Thus, the Cr^{III} and Na^+ centres are bridged by IDA ligands and water molecule O1*W* to form a polymeric structure. An extensive hydrogen-bonding network occurs in the crystal structure (Table 2). While uncoordinated water molecules (O2*W* and O3*W*) form hydrogen bonds with carboxyl groups, as shown in Fig. 1, N—H···O hydrogen bonds exist between imino and carboxyl groups of neighboring Cr complexes (Fig. 2).

Experimental

An ethanol solution (6 ml) containing benzimidazole (0.24 g, 2 mmol) and $CrCl_3·6H_2O$ (0.27 g, 1 mmol) was mixed with an aqueous solution (4 ml) containing IDA (0.13 g, 1 mmol) and Na_2CO_3 (0.10 g, 1 mmol) at room temperature. The mixture was then refluxed for 1 h and filtered. Purple crystals of (I) were obtained from the filtrate after 2 d.

Crystal data

$Na[Cr(C_4H_5NO_4)_2]·1.5H_2O$
$M_r = 364.20$
Monoclinic, $P2_1/c$
$a = 15.5805$ (15) Å
$b = 16.8464$ (16) Å
$c = 10.2030$ (12) Å
$\beta = 90.742$ (2)°
$V = 2677.8$ (5) Å^3
$Z = 8$
$D_x = 1.807$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10968 reflections
$\theta = 2.8$–54.0°
$\mu = 0.94$ mm^{-1}
$T = 295$ (2) K
Plate, purple
0.38 × 0.33 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.702$, $T_{max} = 0.900$
11982 measured reflections
6141 independent reflections
4824 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$
$h = -20 \rightarrow 20$
$k = -21 \rightarrow 21$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.075$
$S = 0.98$
6141 reflections
388 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1

Selected geometric parameters (Å).

Cr1—O13	1.9443 (13)	Na1—O12	2.3437 (16)
Cr1—O11	1.9442 (12)	Na1—O18^{i}	2.3704 (15)
Cr1—O15	1.9585 (13)	Na1—O14^{ii}	2.3818 (16)
Cr1—O17	1.9603 (12)	Na1—O26	2.4017 (15)
Cr1—N11	2.0758 (15)	Na1—O1*W*	2.4131 (17)
Cr1—N12	2.0757 (14)	Na1—O28^{ii}	2.4179 (15)
Cr2—O27	1.9468 (12)	Na2—O28^{iii}	2.3221 (15)
Cr2—O25	1.9528 (13)	Na2—O16	2.3589 (15)
Cr2—O23	1.9550 (13)	Na2—O22^{iv}	2.3659 (17)
Cr2—O21	1.9593 (13)	Na2—O24^{v}	2.3879 (15)
Cr2—N21	2.0686 (14)	Na2—O18^{vi}	2.4376 (17)
Cr2—N22	2.0715 (15)	Na2—O1*W*^{vii}	2.5531 (18)

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···O17^{vi}	0.91	2.18	3.0799 (18)	173
N12—H12···O11^{vi}	0.91	2.08	2.9174 (18	152
N21—H21···O27^{ii}	0.91	2.10	2.9958 (19)	169
N22—H22···O21^{ii}	0.91	2.32	3.1809 (19)	157
O1*W*—H11*W*···O2*W*	0.97	1.83	2.799 (2)	177
O1*W*—H21*W*···O15^{vii}	0.86	2.04	2.895 (2)	174
O2*W*—H12*W*···O25	0.86	2.13	2.975 (2)	167
O2*W*—H22*W*···O3*W*	0.92	1.98	2.847 (3)	158
O3*W*—H13*W*···O23^{viii}	0.87	2.22	2.896 (2)	135
O3*W*—H23*W*···O22	0.87	1.99	2.807 (3)	155

Symmetry codes: (ii) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (vi) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (vii) $1-x, 1-y, 1-z$; (viii) $-x, y-\frac{1}{2}, \frac{1}{2}-z$.

Water H atoms were placed in theoretical positions (Nardelli, 1999) and included in structure-factor calculations with fixed positional parameters and U_{iso} values of 0.05 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.97 Å and N—H =

0.91 Å, and included in the final cycles of refinement in the riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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