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Bis(triethanolamine-*O*,*O*′)nickel(II) diacetate

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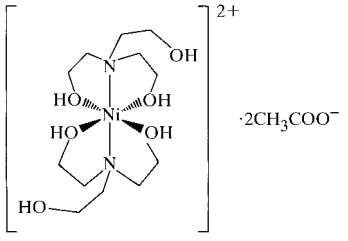
The title compound, $[Ni\{N(CH_2CH_2OH)_3\}_2](CH_3COO)_2$, was prepared and the structure determined. It is isostructural with the copper(II) analogue.

Comment

The Ni^{2+} cation is coordinated by two molecules of triethanolamine, forming an octahedron. This octahedron shows only a slight distortion compared with the Jahn–Teller distortion of Cu^{2+} in the isostructural compound $[Cu\{N(CH_2CH_2OH)_3\}_2](CH_3COO)_2$ (Krabbes *et al.*, 1999). Acetate ions are linked by hydrogen bonds to the triethanolamine hydroxyl groups of the $[Ni\{N(CH_2CH_2OH)_3\}_2]^{2+}$ complex cation. Each acetate ion is linked by two hydrogen bonds to the coordinated hydroxyl groups of the complex cation and by a third hydrogen bond to the free hydroxyl group of a second complex cation species. This causes the formation of chains along the *a* axis. The IR spectrum of the complex, (I), shows



(I)

absorption bands of associated hydroxyl groups at 3260 and 3035 cm^{-1}. Between 3000 and 2400 cm^{-1}, the typical absorption bands of O—H···O-chelates are observed. Valence vibrations of carboxyl groups occur at 1545 (ν_{as}) and 1415 cm^{-1} (ν_s).

Experimental

The synthesis of the title compound was carried out by dissolving nickel(II) acetate tetrahydrate in a tenfold excess of triethanolamine at 423 K. Polycrystalline bis(triethanolamine)nickel(II) acetate precipitated when the solution was cooled down. After removing the excess of triethanolamine the product was washed with acetone. Single crystals of bis(triethanolamine)nickel(II) acetate were obtained by fractional crystallization from a triethanolamine solution. The IR spectrum was recorded using a potassium bromide matrix on a Perkin Elmer FT–IR 2000 spectrometer.

Crystal data

$[Ni(C_6H_{15}NO_3)_2](C_2H_3O_2)_2$	D_x = 1.439 Mg m^{-3}
M_r = 475.18	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 9.123 (1) Å	θ = 12.40–18.71°
b = 13.219 (2) Å	μ = 0.937 mm^{-1}
c = 9.820 (1) Å	T = 296 (2) K
β = 112.17 (6)°	Prism, clear light blue
V = 1096.7 (2) $Å^3$	0.40 × 0.40 × 0.40 mm
Z = 2	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 26.91°
ω–2θ scans	$h = 0 \rightarrow 11$
2524 measured reflections	$k = 0 \rightarrow 16$
2379 independent reflections	$l = -12 \rightarrow 11$
2048 reflections with $I > 2\sigma(I)$	3 standard reflections every 250 reflections
R_{int} = 0.017	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.4638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.077	$\Delta\rho_{max}$ = 0.51 e $Å^{-3}$
S = 0.996	$\Delta\rho_{min}$ = −0.27 e $Å^{-3}$
2379 reflections	
136 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O3^i	2.0636 (12)	Ni1—N1^i	2.1055 (14)
Ni1—O2^i	2.078 (2)		
O3^i—Ni1—O2^i	85.93 (5)	O3^i—Ni1—N1	83.95 (5)
O2^i—Ni1—N1^i	81.88 (5)		

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *HELENA* (Spek, 1992); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); software used to prepare material for publication: *DIAMOND*.

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