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[Tris(2-aminoethyl)amine-κ^3*N*,*N*′,*N*″,*N*‴](L-tyrosinato-κ^2*N*,*O*)nickel(II) iodide dihydrate

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In the title compound, $[Ni(C_9H_{10}NO_3)(C_6H_{18}N_4)]I\cdot 2H_2O$, the Ni^{II} atom is in a slightly distorted octahedral coordination environment. In the crystal structure, extensive hydrogen bonding links molecules into a three-dimensional network.

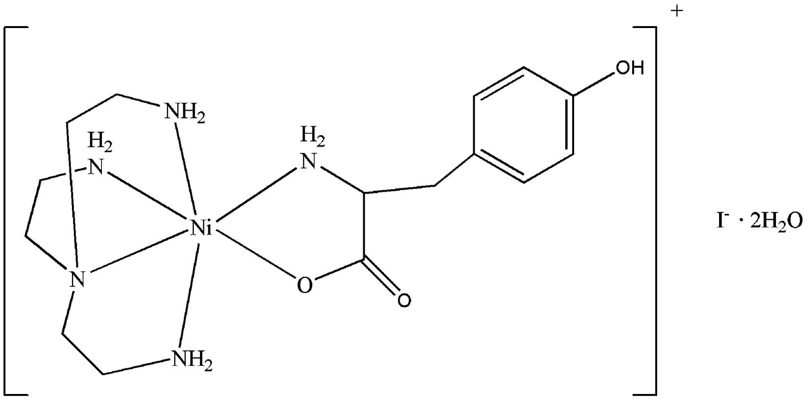
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.037
wR factor = 0.106
Data-to-parameter ratio = 17.4

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

Comment

Amino acids are interesting biological ligands with multiple functional groups. A series of amino acid complexes of Ni^{II} has recently been reported (van der Helm & Hossain, 1969; Campana *et al.*, 1981; Antolini *et al.*, 1982; Demaret & Mercier, 1983; Shvelashvili *et al.*, 1984; Teoh *et al.*, 1987; Baidya *et al.*, 1991; Wang *et al.*, 2002; 2004).



(I)

In the title molecular structure, (I), the Ni^{II} atom is coordinated by four N atoms from a tetradendate tren (tren is tren is 2,2′,2″-triaminotriethylamine) ligand, one carboxylate O atom and the amino N atom of an L-tyrosinate ligand (Fig. 1). The coordination geometry is slightly distorted ocahedral. Selected bond lengths and angles are given in Table 1.

In the crystal structure, intermolecular N—H⋯I, N—H⋯O, O—H⋯O, O—H⋯N and O—H⋯I hydrogen bonds link ions and solvent molecules into a three-dimensional network (Table 2 and Fig. 2). In addtion, the details of two significant H⋯π(arene) interactions are listed in Table 2.

Experimental

L-Tyrosine (0.18 g, 1 mmol) was added to an aqueous solution (10 ml) of tren (0.15 g, 1 mmol). A freshly prepared 0.1 mol l^{-1} NaOH solution was added until pH = 9 was achieved. An aqueous solution (10 ml) of $Ni(NO_3)_2\cdot 6H_2O$ (0.29 g, 1 mmol) was then added and stirred for 2 h. The solution slowly changed to purple. This resulting solution was treated with KI (0.16 g, 1 mmol), cooled to room temperature and filtered. The solution was maintained at room temperature. Purple block-shaped crystals suitable for X-ray analysis were obtained after several days in 55% yield.

Crystal data

$[Ni(C_9H_{10}NO_3)(C_6H_{18}N_4)]I\cdot 2H_2O$	$Z = 2$
$M_r = 548.05$	$D_x = 1.703$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 10.2197$ (14) Å	$\mu = 2.39$ mm^{-1}
$b = 10.3097$ (14) Å	$T = 293$ (2) K
$c = 10.2801$ (14) Å	Block, purple
$\beta = 99.415$ (2)°	0.20 × 0.20 × 0.10 mm
$V = 1068.5$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	6707 measured reflections
φ and ω scans	4255 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	4056 reflections with $I > 2\sigma(I)$
$T_{min} = 0.647$, $T_{max} = 0.796$	$R_{int} = 0.069$
	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.0892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.106$	$\Delta\rho_{max} = 0.74$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.67$ e Å^{-3}
4255 reflections	Absolute structure: Flack (1983), 1697 Friedel pairs
244 parameters	Flack parameter: 0.02 (2)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—N5	2.079 (4)	Ni1—N3	2.099 (4)
Ni1—N1	2.081 (4)	Ni1—N2	2.138 (4)
Ni1—O1	2.089 (3)	Ni1—N4	2.153 (4)
N5—Ni1—N1	176.00 (17)	O1—Ni1—N2	89.36 (16)
N5—Ni1—O1	79.89 (15)	N3—Ni1—N2	95.40 (17)
N1—Ni1—O1	97.09 (14)	N5—Ni1—N4	100.60 (17)
N5—Ni1—N3	98.77 (16)	N1—Ni1—N4	81.62 (17)
N1—Ni1—N3	84.46 (16)	O1—Ni1—N4	84.36 (16)
O1—Ni1—N3	175.16 (17)	N3—Ni1—N4	91.34 (17)
N5—Ni1—N2	95.16 (16)	N2—Ni1—N4	161.70 (18)
N1—Ni1—N2	82.13 (16)	C7—O1—Ni1	117.0 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*OB*···I1	0.82	2.73	3.475 (4)	151
O3—H3···O4	0.82	1.90	2.687 (6)	160
O5—H5*OB*···O2	0.82	1.89	2.707 (6)	179
N5—H5*D*···O3^{i}	0.90	2.50	3.219 (6)	138
N5—H5*C*···O5^{ii}	0.90	2.06	2.937 (7)	164
N4—H4*C*···I1^{iii}	0.90	3.00	3.851 (5)	159
N3—H3*C*···I1^{i}	0.90	3.00	3.756 (4)	143
O5—H5*OA*···I1^{iv}	0.83	2.66	3.489 (4)	179
O4—H4*OA*···O2^{v}	0.82	1.94	2.762 (6)	180
N2—H2*C*···*Cg*1	0.90	2.43	3.210 (4)	144
C3—H3*B*···*Cg*2	0.97	2.78	3.695 (5)	158

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

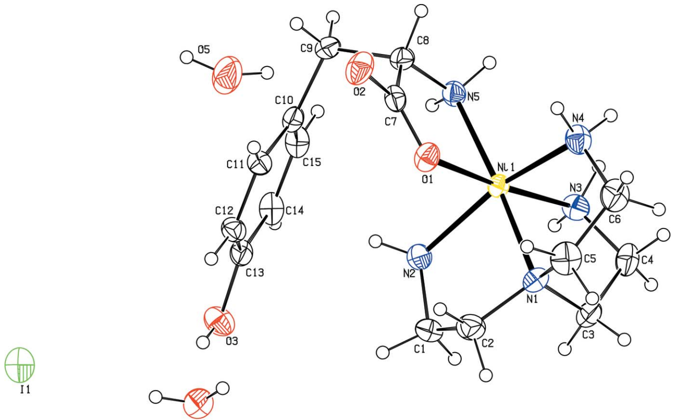


Figure 1
View of the title molecular structure, showing 50% probability displacement ellipsoids and H atoms as small spheres.

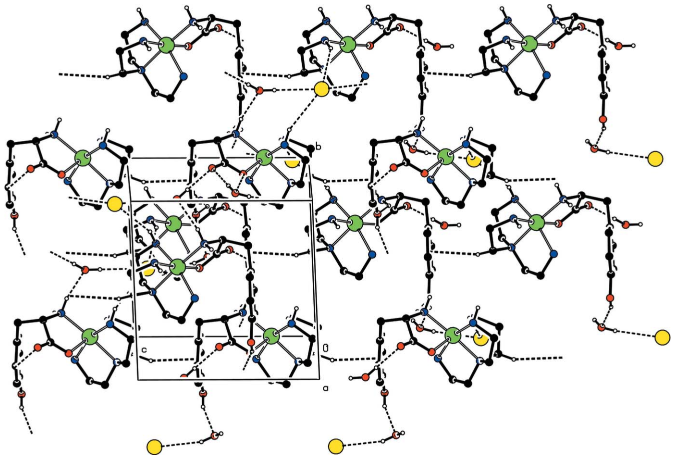


Figure 2
View of part of the crystal structure of (I), showing hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

All H atoms bonded to C and N atoms, and the hydroxyl O atom (O3) were placed in calculated positions, with C—H = 0.93–0.97 Å, N—H = 0.90 Å or O—H = 0.82 Å, and included in a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}(O)$. The H atoms bonded to solvent water O atoms were placed in positions that gave theoretically ideal hydrogen bonds based on the most likely O···O contacts. They were then refined in a riding-model approximation, with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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