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## Sodium hydrogen nitrilotriacetate dihydrate

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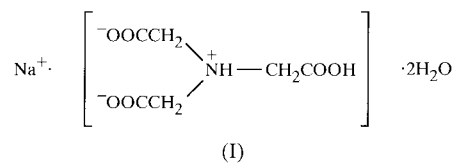
Data validation number: IUC0000238

In the title compound,  $\text{Na}^+ \cdot \text{C}_6\text{H}_8\text{NO}_6^- \cdot 2\text{H}_2\text{O}$ , the sodium ion is coordinated in a distorted octahedral manner by two carboxylate O atoms and two water O atoms. Each of these water molecules bridges two adjacent Na ions, resulting in two four-membered rings of the type Na–O–Na–O.

### Comment

Recently, much attention has been paid to nitrilotriacetate acid (NTA), a multidentate complexing ligand with high specificity for various polyvalent metal ions. The trivalent NTA anion normally coordinates with alkali earth and transition metal ions as tetradentate ligands, binding through an N atom and three acetate O atoms to the metal (Barnett & Uchtman, 1979; Kaneyoshi *et al.*, 1999). However, for a few complexes, NTA is hexadentate or heptadentate (Martin & Jacobson, 1972). The structure of trisodium nitrilotriacetate has been proposed as polymeric with seven O atoms and one N atom coordinated to three sodium ions (Dely, 1967).

The crystal structure of the title compound, (I), contains sodium ions chelated by NTA molecules *via* two Na–O bonds [2.436 (2) and 2.345 (2) Å]. The observed Na–O bond distances are within the range 2.28–2.67 Å, reported by Dely (1967). The O–Na–O angle is 88.35 (5)°. Two water molecules are involved in each molecular unit and bridge two adjacent sodium ions, with one water O atom coordinated to Na and Na<sup>i</sup>, and the other to Na and Na<sup>ii</sup> [symmetry codes: (i)  $-x, 1-y, -z$ ; (ii)  $1-x, 1-y, -z$ ]. The four Na–OW bond distances are in the range 2.345 (2)–2.561 (2) Å and the two OW–Na–OW angles are 91.36 (6) and 88.04 (6)°. The geometry around the sodium ion can be described as slightly distorted octahedral. The infinite crystal network is formed *via* four-membered Na–OW–Na–OW rings between two layers and *via* hydrogen bonds between two adjacent molecular units in a given layer.



### Experimental

The title compound was obtained in the attempted preparation of an erbium–NTA complex, by mixing 0.50 M Er<sup>III</sup> and 0.50 M Na<sub>2</sub>NTA aqueous solutions in a 1:4 molar ratio. The pH of the solution was adjusted to 4.5. Colourless microcrystals of the title compound were obtained by slow evaporation.

### Compound (I)

#### Crystal data

$\text{Na}^+ \cdot \text{C}_6\text{H}_8\text{NO}_6^- \cdot 2\text{H}_2\text{O}$   
 $M_r = 249.16$   
Orthorhombic, *Pbca*  
 $a = 5.8620$  (19) Å  
 $b = 12.3986$  (16) Å  
 $c = 26.854$  (3) Å  
 $V = 1951.8$  (7) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.696$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 42 reflections  
 $\theta = 6.75$ – $12.57^\circ$   
 $\mu = 0.193$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Needle, colourless  
 $0.40 \times 0.15 \times 0.10$  mm

#### Data collection

Bruker P4 diffractometer  
 $2\theta/\omega$  scans  
Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)  
 $T_{\min} = 0.873$ ,  $T_{\max} = 0.981$   
4474 measured reflections  
2239 independent reflections  
1731 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$   
 $\theta_{\max} = 27.50^\circ$   
 $h = -7 \rightarrow 7$   
 $k = -16 \rightarrow 16$   
 $l = -34 \rightarrow 34$   
3 standard reflections  
every 97 reflections  
intensity decay: 3.0%

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.109$   
 $S = 1.047$   
2239 reflections  
169 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.3629P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.31$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °) for (I).

Na1–O3	2.3450 (15)	Na1–O1	2.4362 (16)
Na1–OW1	2.3778 (16)	Na1–OW2	2.4712 (18)
Na1–OW1 <sup>i</sup>	2.4271 (18)	Na1–OW2 <sup>ii</sup>	2.561 (2)
O3–Na1–OW1	92.86 (6)	O3–Na1–OW2 <sup>ii</sup>	98.61 (6)
O3–Na1–OW1 <sup>i</sup>	83.74 (6)	OW1–Na1–OW2 <sup>ii</sup>	90.38 (6)
OW1–Na1–OW1 <sup>i</sup>	88.04 (6)	OW1 <sup>i</sup> –Na1–OW2 <sup>ii</sup>	177.24 (6)
O3–Na1–O1	88.35 (5)	O1–Na1–OW2 <sup>ii</sup>	93.69 (6)
OW1–Na1–O1	175.53 (6)	OW2–Na1–OW2 <sup>ii</sup>	91.31 (6)
OW1 <sup>i</sup> –Na1–O1	87.81 (6)	Na1–OW1–Na1 <sup>i</sup>	91.96 (6)
O3–Na1–OW2	168.83 (7)	Na1–OW2–Na1 <sup>ii</sup>	88.69 (6)
OW1–Na1–OW2	81.89 (6)	C2–O1–Na1	115.32 (12)
OW1 <sup>i</sup> –Na1–OW2	86.22 (6)	C4–O3–Na1	163.21 (13)
O1–Na1–OW2	96.17 (6)		

Symmetry codes: (i)  $-x, 1-y, -z$ ; (ii)  $1-x, 1-y, -z$ .

Positional parameters of H atoms bonded to C atoms were calculated geometrically. The H atoms bonded to the N and O atoms were observed from difference syntheses and refined isotropically. The N—H and O—H bond lengths are 0.92 (2) Å and 0.81 (4)–0.90 (3) Å, respectively.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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