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## Key indicators

Single-crystal X-ray study  
 $T = 299$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.093  
Data-to-parameter ratio = 13.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

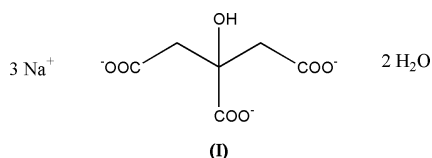
## Trisodium citrate dihydrate

From a solution containing uranyl nitrate and sodium citrate, single crystals of trisodium citrate dihydrate,  $3\text{Na}^+\cdot\text{C}_6\text{H}_5\text{O}_7^{3-}\cdot 2\text{H}_2\text{O}$ , were obtained. The structure consists of a complex network of citrate and sodium ions. Additionally, hydrogen bonds between the citrate ions and the water of crystallization are formed.

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## Comment

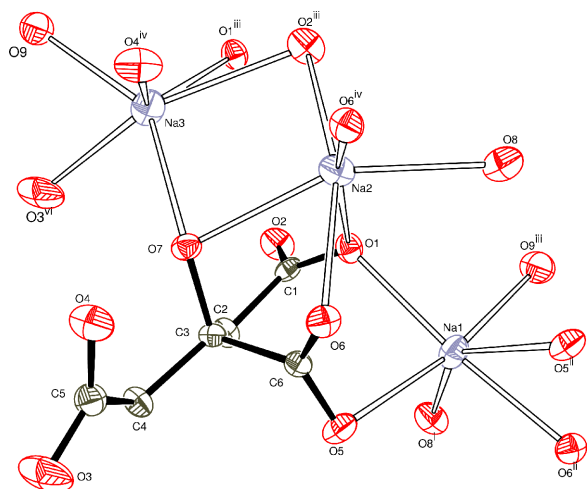
Citric acid is a tricarboxylic acid, which can undergo different degrees of deprotonation and thus can form different reaction products with alkali hydroxide, depending on the molar ratio. Additionally, the amount of water of crystallization may vary depending on the stoichiometry and concentration of the different species in the reaction medium. The unit cells and space groups of a number of sodium and potassium citrates have been known for a long time (Burns & Iball, 1954). However, no structure determination of a sodium citrate dihydrate has been undertaken. Later, the structures of two other hydrates of sodium citrate were determined, *viz.* sodium dihydrogen citrate (Glusker *et al.*, 1965) and trisodium citrate 5.5-hydrate (Viostat *et al.*, 1986).



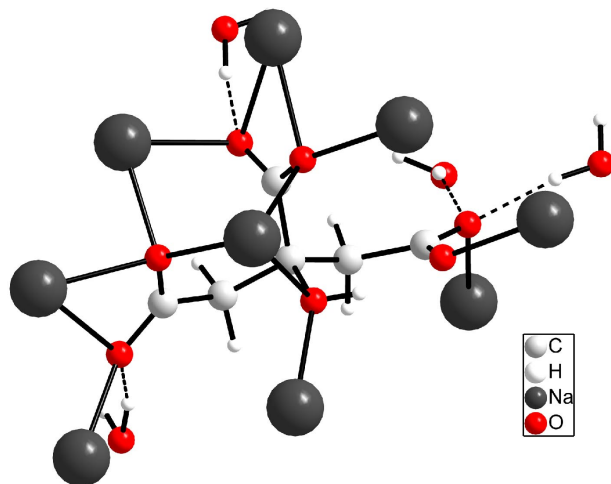
In our investigations of the uranyl/citrate system, we obtained single crystals of trisodium citrate dihydrate, (I), whose structure has been determined. It contains one citrate anion, whose geometry is unexceptional, and three  $\text{Na}^+$  ions in the asymmetric unit (Fig. 1). The  $\text{Na}^+$  ions are coordinated by both citrate ions and water molecules, yielding a coordination number of 6, with rather irregular coordination polyhedra (Fig. 1). Each citrate ion coordinates to nine  $\text{Na}^+$  ions as a bridging ligand, yielding a complex three-dimensional network. Additionally, the water ligands form hydrogen bonds to some of the carboxyl O atoms (Fig. 2). The coordination of the citrate ion is shown in Fig. 1, while Fig. 3 shows the unit-cell contents.

## Experimental

To a solution of uranyl nitrate hexahydrate and trisodium citrate in a molar ratio of 1:3, sodium hydroxide was added until a pale-yellow product started to precipitate. From this solution, colourless crystals of the title compound were obtained upon standing for one month.

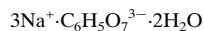

**Figure 1**

The citrate ion and the three Na<sup>+</sup> ions with their complete coordination environments in the structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i)  $x, 1 - y, z - \frac{1}{2}$ ; (ii)  $1 - x, 1 - y, -z$ ; (iii)  $\frac{1}{2} - x, \frac{1}{2} - y, -z$ ; (iv)  $1 - x, y, \frac{1}{2} - z$ ; (v)  $1 - x, -y, -z$ .]


**Figure 2**

The citrate ion and the surrounding Na<sup>+</sup> ions and water molecules. Hydrogen bonds are shown as dashed lines.

#### Crystal data


 $M_r = 294.10$ 

 Monoclinic,  $C2/c$ 
 $a = 15.7044 (4) \text{ \AA}$ 
 $b = 12.5010 (4) \text{ \AA}$ 
 $c = 11.2837 (4) \text{ \AA}$ 
 $\beta = 103.5841 (13)^\circ$ 
 $V = 2153.26 (12) \text{ \AA}^3$ 
 $Z = 8$ 
 $D_x = 1.814 \text{ Mg m}^{-3}$ 

 Mo  $K\alpha$  radiation

Cell parameters from 3843 reflections

 $\theta = 4.5\text{--}27.5^\circ$ 
 $\mu = 0.27 \text{ mm}^{-1}$ 
 $T = 299 \text{ K}$ 

Cuboid, colourless

 $0.20 \times 0.15 \times 0.10 \text{ mm}$ 

#### Data collection

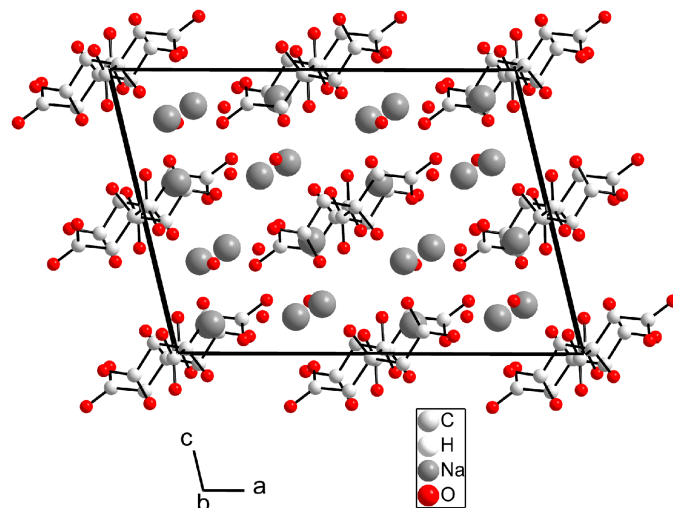
Bruker–Nonius KappaCCD diffractometer

 $\omega$  scans

Absorption correction: none

8459 measured reflections

2451 independent reflections

 1643 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.055$ 
 $\theta_{\text{max}} = 27.5^\circ$ 
 $h = -17 \rightarrow 20$ 
 $k = -14 \rightarrow 16$ 
 $l = -14 \rightarrow 12$ 

**Figure 3**

The unit cell contents, viewed along  $b$ . H atoms have been omitted.

#### Refinement

 Refinement on  $F^2$ 
 $R[F^2 > 2\sigma(F^2)] = 0.040$ 
 $wR(F^2) = 0.093$ 
 $S = 1.02$ 

2451 reflections

178 parameters

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0385P)^2$ 
 $+ 0.6276P]$ 

 where  $P = (F_o^2 + 2F_c^2)/3$ 
 $(\Delta/\sigma)_{\text{max}} < 0.001$ 
 $\Delta\rho_{\text{max}} = 0.43 \text{ e \AA}^{-3}$ 
 $\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$ 
**Table 1**

 Selected geometric parameters ( $\text{\AA}$ ).

Na1—O8 <sup>i</sup>	2.3404 (18)	Na2—O6	2.3819 (15)
Na1—O1	2.3442 (16)	Na2—O8	2.450 (2)
Na1—O6 <sup>ii</sup>	2.3621 (16)	Na2—O1	2.4588 (16)
Na1—O9 <sup>iii</sup>	2.3819 (17)	Na2—Na3	3.3241 (13)
Na1—O5	2.4627 (17)	Na2—Na2 <sup>iv</sup>	3.5644 (15)
Na1—O5 <sup>ii</sup>	2.5492 (18)	Na2—Na3 <sup>iii</sup>	4.2172 (12)
Na1—C6 <sup>ii</sup>	2.775 (2)	Na3—O4 <sup>iv</sup>	2.3346 (17)
Na1—Na2 <sup>i</sup>	3.3240 (12)	Na3—O7	2.3947 (15)
Na1—Na3 <sup>iii</sup>	3.4123 (11)	Na3—O1 <sup>iii</sup>	2.3999 (15)
Na1—Na1 <sup>ii</sup>	3.4358 (16)	Na3—O9	2.4013 (19)
Na2—O2 <sup>iii</sup>	2.3163 (16)	Na3—O2 <sup>iii</sup>	2.6184 (17)
Na2—O6 <sup>iv</sup>	2.3342 (16)	Na3—O3 <sup>v</sup>	2.781 (2)

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

**Table 2**

 Hydrogen-bonding geometry ( $\text{\AA}, ^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O7—H7 <sup>..</sup> ·O4	0.82 (2)	1.85 (2)	2.6072 (19)	153 (2)
O8—H8A <sup>..</sup> ·O5 <sup>vi</sup>	0.803 (15)	2.030 (16)	2.820 (2)	168 (3)
O8—H8B <sup>..</sup> ·O3 <sup>vi</sup>	0.840 (15)	1.920 (16)	2.755 (2)	173 (2)
O9—H9A <sup>..</sup> ·O3 <sup>v</sup>	0.808 (15)	1.974 (17)	2.706 (2)	150 (2)
O9—H9B <sup>..</sup> ·O2 <sup>vii</sup>	0.810 (16)	1.953 (16)	2.762 (2)	176 (3)

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

H atoms attached to carbon were positioned geometrically ( $C\text{—}H = 0.97 \text{ \AA}$ ) and refined in the riding-model approximation, with  $U_{\text{iso}}$  equal to  $1.2U_{\text{eq}}$  of the carrier atom. The geometry of the water

molecules were restrained to a reasonable chemical model [O—H = 0.82 (1) Å and H···H=1.37 (1) Å]. The H-atom coordinates were then allowed to refine, with  $U_{\text{iso}}$  equal to  $1.2U_{\text{eq}}$  of the O atom.

Data collection: *KappaCCD Software* (Nonius, 1997); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *maXus* (Mackay *et al.*, 1997).

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