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Sodium isocyanurate monohydrate

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The crystal structure of the title compound, $Na^+\cdot C_3H_2N_3O_3^-\cdot H_2O$, contains double chains of edge-shared distorted NaO_6 octahedra propagating in the [100] direction. The double chains are linked by the isocyanurate anions.

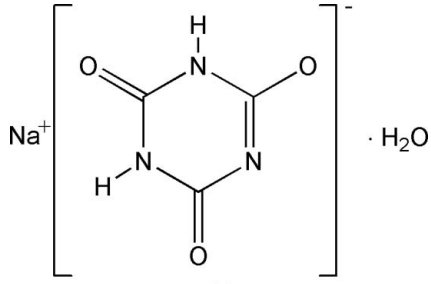
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(N–C) = 0.001 Å
R factor = 0.036
wR factor = 0.113
Data-to-parameter ratio = 19.7

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

Comment

The title compound, (I) (Fig. 1), appeared as an intermediate in our study of carbon nitrides and hitherto has not been reported. We report here its preparation and crystal structure.



(I)

In the structure of (I), all atoms are approximately on the (101) plane, except for the water molecules, which are located above or below the plane. The structure contains double chains of edge-shared distorted NaO_6 octahedra propagating in the [100] direction. Four O atoms of each octrahedron come from the isocyanurate anions, and the other two are from two water molecules. The double chains are linked to each other by the isocyanurate anions (Fig. 2). The Na—O bond lengths range from 2.3412 (10) to 2.6064 (10) Å (Table 1). This indicates the irregularity of the NaO_6 octahedra. The intrachain Na···Na separation along the a direction is equal to the length of the a axis [3.5987 (1) Å].

Experimental

Melamine (0.315 g, 0.025 mol), cyanuric chloride (0.922 g, 0.05 mol) and sodium chloride (0.5 g, 0.009 mol) were put into a 30 ml Teflon-lined autoclave containing water (20 ml) as solvent. The autoclave was heated and kept at 493 K for 3 h. After natural cooling to room temperature, colorless needle-like crystals of (I) were obtained.

Crystal data

$Na^+\cdot C_3H_2N_3O_3^-\cdot H_2O$
M_r = 169.08
Triclinic, $P\overline{1}$
a = 3.5987 (1) Å
b = 9.1257 (1) Å
c = 9.2311 (1) Å
α = 91.139 (1)°
β = 99.159 (1)°
γ = 91.535 (1)°
V = 299.09 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 (2) K
0.21 × 0.11 × 0.09 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.90, T_{max} = 0.98
6793 measured reflections
2163 independent reflections
1831 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.113
S = 1.05
2163 reflections
110 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na—O4	2.3412 (10)	Na—O1^{ii}	2.3969 (8)
Na—O4^{i}	2.3587 (10)	Na—O3^{iii}	2.4980 (9)
Na—O3	2.3882 (9)	Na—O3^{iv}	2.6064 (10)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···N3^{v}	0.85	2.10	2.8434 (12)	146
O4—H4B···O2^{vi}	0.85	1.96	2.7788 (12)	163
N1—H1···O2^{vii}	0.901 (18)	1.896 (18)	2.7966 (12)	176.6 (15)
N2—H2···O1^{viii}	0.888 (19)	1.981 (19)	2.8530 (11)	167.1 (17)

Symmetry codes: (v) $x-1, y, z$; (vi) $-x+1, -y+1, -z$; (vii) $-x+2, -y+2, -z$; (viii) $-x+1, -y+2, -z+1$.

H atoms bonded to N atoms were located in a difference Fourier map and their positions and isotropic displacement parameters were refined freely. The positions of the H atoms of the water molecule were obtained by using the *XHYDEX* program (Orpen, 1980) and refined using a riding model; their U_{iso}(H) values were refined freely.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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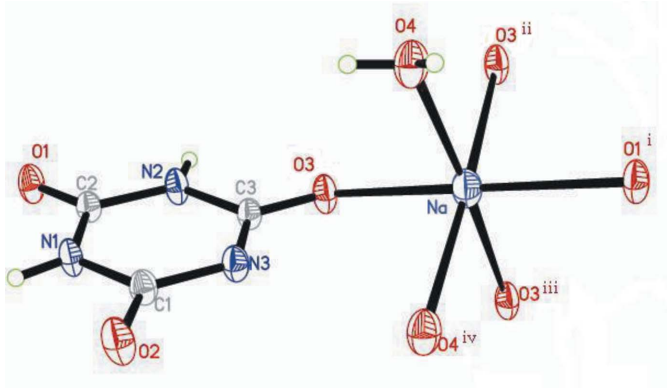

Figure 1
The asymmetric unit of (I), extended to show the complete Na coordination. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -y+1$; (iv) $x+1, y, z$.]

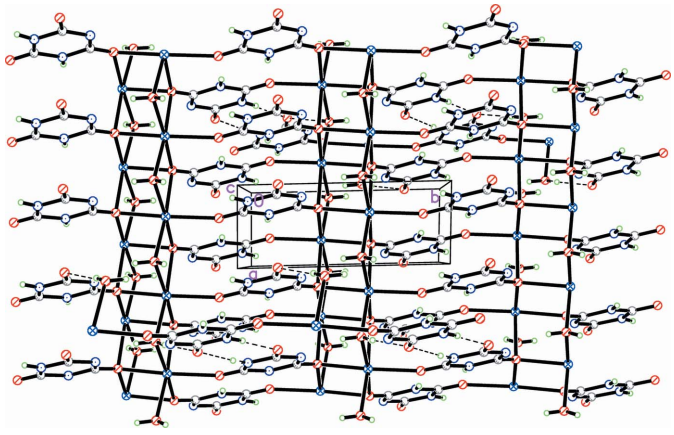

Figure 2
The crystal packing of (I). Dashed lines indicate hydrogen bonds.

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