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catena-Poly[2,4,6-triamino-1,3,5-triazin-1-ium [[aqua(pyridine-2,6-dicarboxylato-κ^3O,N,O')-bismuthate(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4O,N,O':O'$]]

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The reaction of $Bi(NO_3)_3{\cdot}5H_2O$ with a 1:2 molecular complex of pyridine-2,6-dicarboxylic acid ($pydcH_2$) and 2,4,6-triamino-1,3,5-triazine (tata) in aqueous solution leads to formation of the title compound, $(C_3H_7N_6)[Bi(C_7H_3NO_4)_2(H_2O)]$. The Bi^{III} atom is octacoordinated by two tridentate $pydc^{2-}$ ligands, one O atom of a water molecule and one O atom from a Bi—O—Bi bridge. Extensive O—H···O and N—H···O hydrogen bonding exists between the anionic polymers and the $tataH^+$ cations.

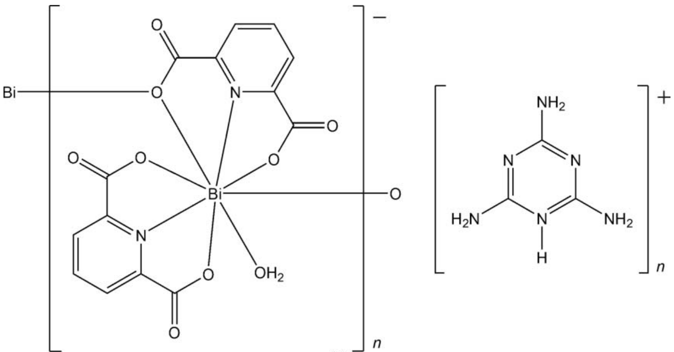
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.026
wR factor = 0.066
Data-to-parameter ratio = 15.4

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

Comment

We have previously reported a number of proton transfer compounds (Aghabozorg, Ghadermazi & Attar Gharamaleki, 2006; Sheshmani *et al.*, 2006; Sharif *et al.*, 2006) and some mono- and dinuclear complexes of these with metal cations (Aghabozorg, Ghasemikhah *et al.*, 2006; Aghabozorg, Aghajani & Sharif, 2006; Aghajani *et al.*, 2006; Sharif *et al.*, 2006). The title compound, (I), is a polymeric Bi^{III} complex containing pyridine-2,6-dicarboxylate ($pydc^{2-}$) ligands and protonated 2,4,6-triamino-1,3,5-triazine ($tataH^+$) counter-ions.



(I)

The crystal structure of (I) contains anionic $\{Bi(C_7H_3NO_4)_2(H_2O)\}_n^{n-}$ polymers (Fig. 1). Each Bi^{III} atom is octacoordinated by two tridentate $pydc^{2-}$ ligands, one O atom of a water molecule and one O atom from a Bi—O8—Bi bridge (Table 1). The bridging carboxylate group exhibits an additional Bi(x, $-y-\frac{1}{2}$, $z+\frac{1}{2}$)···O6 contact of 3.366 (4) Å so that it approaches a highly asymmetric bidentate binding mode. The Bi—O bond distances (Table 1) span a broad range, with short distances (Bi—O1^{i} and Bi—O6) lying opposite longer distances (Bi—O8 and Bi—O9).

The anionic polymers lie in layers parallel to the *ac* planes, with the $tataH^+$ cations between them (Fig. 2). The $tataH^+$ cations form pairs, with their planes parallel and separated by 3.27 (1) Å, indicating a π–π stacking interaction between

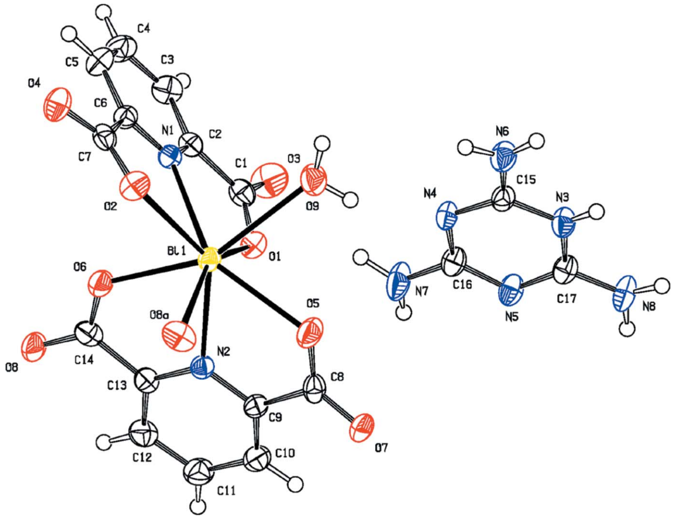


Figure 1
The asymmetric unit, together with atom O8a to complete the coordination of Bi1. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms. Atom O8a is generated by the symmetry code (x, $-\frac{1}{2} - y$, $-\frac{1}{2} + z$).

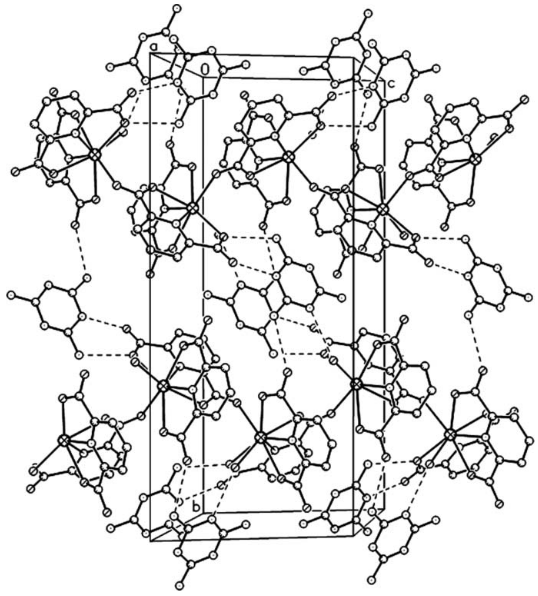


Figure 2
Packing diagram of (I) showing $\{Bi(C_7H_3NO_4)_2(H_2O)\}_n^{n-}$ polymers in layers parallel to the ac planes, with pairs of tataH$^+$ cations between them. H atoms have been omitted. Dashed lines denote hydrogen bonds.

them. Extensive O—H···O and N—H···O hydrogen bonding (Table 2) exists between the anionic polymers and the tataH$^+$ cations.

Experimental

A solution of $Bi(NO_3)_3\cdot5H_2O$ (0.058 g, 0.083 mmol) in water (5 ml) was added to a stirred aqueous solution (10 ml) of a 1:2 molecular complex of pyridine-2,6-dicarboxylic acid and 2,4,6-triamino-1,3,5-triazine (0.070 g, 0.167 mmol). The volume of the resulting suspension was increased by adding 50 ml of water, and the clear solution was stirred at 313–323 K for 2 h. Colourless single crystals of (I) were collected from the solution after standing at room temperature for a few days.

Crystal data

$(C_3H_7N_6)[Bi(C_7H_3NO_4)_2(H_2O)]$
M_r = 684.35
Monoclinic, $P2_1/c$
a = 9.3948 (19) Å
b = 23.351 (5) Å
c = 9.950 (2) Å
β = 111.88 (3)°
V = 2025.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.78 mm^{-1}
T = 293 (2) K
0.35 × 0.20 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.195, T_{max} = 0.645
5152 measured reflections
4871 independent reflections
3715 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
2 standard reflections every 98 reflections intensity decay: 2.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.066
S = 1.03
4871 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Bi1—O1	2.333 (3)	Bi1—O5	2.486 (3)
Bi1—O6	2.374 (3)	Bi1—O2	2.535 (3)
Bi1—N1	2.448 (3)	Bi1—O8^{i}	2.586 (3)
Bi1—N2	2.452 (3)	Bi1—O9	2.618 (3)
O1—Bi1—N1	67.22 (11)	O6—Bi1—O2	76.66 (11)
O6—Bi1—N2	66.66 (11)	N1—Bi1—O2	64.84 (11)
O1—Bi1—O5	80.24 (12)	O1—Bi1—O9	70.48 (11)
O6—Bi1—O5	130.03 (11)	O6—Bi1—O9	149.91 (11)
N2—Bi1—O5	64.22 (11)	O5—Bi1—O9	73.39 (11)
O1—Bi1—O2	131.96 (11)	O2—Bi1—O9	95.40 (11)

Symmetry code: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3N···O7^{ii}	0.90	1.84	2.686 (5)	156
N6—H6A···O4^{iii}	0.90	1.99	2.892 (5)	174
N6—H6B···O3^{iv}	0.90	2.51	3.285 (6)	144
N7—H7A···O1	0.90	2.17	3.001 (5)	152
N7—H7B···O1^{v}	0.90	2.33	3.190 (5)	160
N8—H8A···O5^{ii}	0.90	1.97	2.842 (5)	162
N8—H8B···O2^{vi}	0.90	2.14	3.013 (5)	162
O9—H9A···N4	0.85	2.09	2.898 (5)	159
O9—H9B···O4^{iii}	0.85	2.14	2.810 (5)	135

Symmetry codes: (ii) $-x+1, -y, -z+2$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, y, z-1$; (v) $-x+1, -y, -z+3$; (vi) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$.

H atoms bound to C atoms were placed in calculated positions and refined using a riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms bound to N and O were located in difference Fourier maps. The N—H and O—H distances were normalized to 0.90 and 0.85 Å, respectively, and the H atoms were subsequently refined as riding with U_{iso}(H) = 1.2U_{eq}(ON).

m1600 Sharif *et al.* • $(C_3H_7N_6)[Bi(C_7H_3NO_4)_2(H_2O)]$ *Acta Cryst.* (2007). E**63**, m1599–m1601

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms, 1995); program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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