

catena-Poly[[diaqualithium(I)]- μ -[9*H*-purine-2,6(1*H*,3*H*)-dionato-O²:N⁷]]

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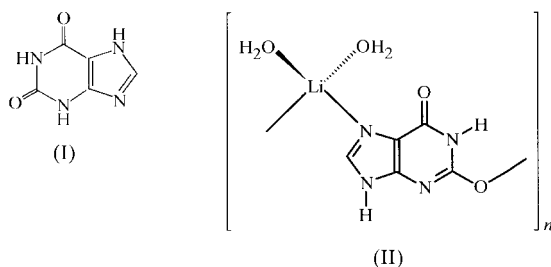
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In the title compound, $[\text{Li}(\text{C}_5\text{H}_3\text{N}_4\text{O}_2)(\text{H}_2\text{O})_2]_n$, the coordination geometry about the Li^+ ion is distorted tetrahedral and the Li^+ ion is bonded to N and O atoms of adjacent ligand molecules forming an infinite polymeric chain with Li—O and Li—N bond lengths of 1.901 (5) and 2.043 (6) Å, respectively. Tetrahedral coordination at the Li^+ ion is completed by two *cis* water molecules [Li—O 1.985 (6) and 1.946 (6) Å]. The crystal structure is stabilized both by the polymeric structure and by a hydrogen-bond network involving N—H...O, O—H...O and O—H...N hydrogen bonds.

Comment

3,7-Dihydro-1*H*-purine-2,6-dione, (I), known as xanthine, is a well known metabolite of purine bases, guanine and adenine, derived from hypoxanthine by xanthine oxidase or from



guanine by guanase (Martin, 1983). Xanthine is further converted to the final metabolite, namely uric acid. In xanthinurea, crystalline xanthine is found as a constituent of

urinary calculi or in muscle tissue as a crystalline alkaline salt of uric acid in hyperuricemia or gout. Up until now, structures of chelate compounds of xanthine with the transition metal ions Cu^{II} , Zn^{II} , Co^{III} , Tl^{III} and Hg^{I} have been determined (Dubler *et al.*, 1992). However structural information on compounds with alkaline or alkaline earth metals is rare. The only structurally characterized compound is the sodium salt of xanthine (Mizuno *et al.*, 1969), in which each Na^+ cation is surrounded by six water molecules and each xanthine anion participates in hydrogen bonds without direct coordination to the metal ions.

In order to clarify the coordination modes of chelate compounds of xanthine with alkaline metals, we have analyzed the 1:1 complex, (II), of the Li^+ ion with xanthine.

The complex contains a monoanionic ligand in which deprotonation of the xanthine has taken place at the N3—H imino group (see Fig. 1). The coordination geometry about the Li^+ ion is distorted tetrahedral (Table 1), with the Li^+ ion bonded to N7 of one ligand and O1 of a symmetry-related ligand to yield an infinite-chain structure. This polymeric coordination mode has not been seen in any other metal compound of xanthine. The O1—C2 bond distance of 1.268 (4) Å is significantly longer than the standard C=O double-bond distance of 1.20 Å. This suggests the presence of some negative charge at the O1 atom of the xanthine anion. The Li^+ ion is also bonded to two water O atoms.

The crystal structure is also stabilized by a network of N—H...O, O—H...O and O—H...N hydrogen bonds, as detailed in Table 2. No stacking interactions between the xanthine ligands are observed.

Experimental

The crystal used for analysis was obtained by slow evaporation from a 50% ethanol–water solution of a mixture containing xanthine and lithium hydroxide (1:1) at room temperature.

Crystal data

 $[\text{Li}(\text{C}_5\text{H}_3\text{N}_4\text{O}_2)(\text{H}_2\text{O})_2]$
 $M_r = 194.08$

 Triclinic, *P1*
 $a = 5.4017$ (5) Å

 $b = 8.3903$ (7) Å

 $c = 4.6325$ (4) Å

 $\alpha = 102.237$ (7)°

 $\beta = 93.676$ (8)°

 $\gamma = 104.154$ (6)°

 $V = 197.46$ (3) Å³
 $Z = 1$
 $D_x = 1.632$ Mg m⁻³

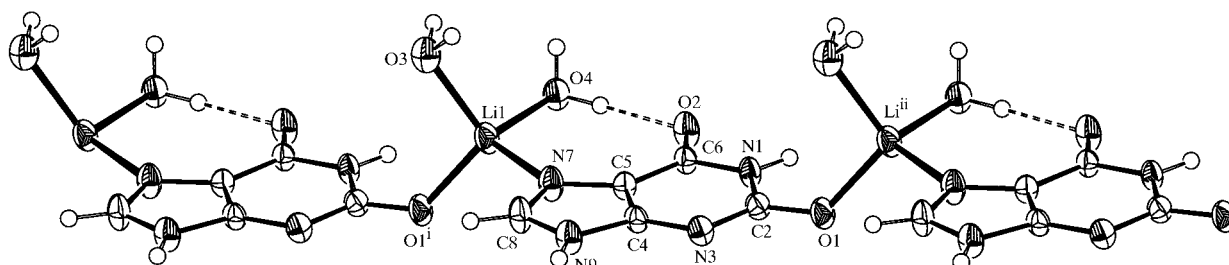
 Mo *K*α radiation

Cell parameters from 25 reflections

 $\theta = 12.70$ – 14.45 °

 $\mu = 0.138$ mm⁻¹
 $T = 293$ (2) K

Prism, colorless

 $0.13 \times 0.12 \times 0.10$ mm

Figure 1

ORTEP (Johnson, 1976) drawing of (II) with the atomic numbering scheme. Ellipsoids for non-H atoms correspond to 50% probability. The symmetry codes are as in Table 1.

Data collection

Rigaku AFC-5R diffractometer	$h = -7 \rightarrow 7$
ω -2 θ scans	$k = -10 \rightarrow 10$
1015 measured reflections	$l = 0 \rightarrow 6$
903 independent reflections	3 standard reflections
722 reflections with $I > 2\sigma(I)$	every 150 reflections
$R_{\text{int}} = 0.018$	intensity decay: 0.07%
$\theta_{\text{max}} = 27.5^\circ$	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R(F) = 0.032$	
$wR(F^2) = 0.096$	
$S = 0.868$	$w = 1/[\sigma^2(F_o^2)]$
903 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
140 parameters	$\Delta\rho_{\text{max}} = 0.175 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.221 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Li1—O1 ⁱ	1.901 (5)	Li1—O4	1.946 (6)
Li1—O3	1.985 (6)	Li1—N7	2.043 (6)
O1 ⁱ —Li1—O3	105.5 (3)	O3—Li1—N7	114.9 (3)
O1 ⁱ —Li1—O4	120.9 (3)	C2—O1—Li1 ⁱⁱ	129.8 (3)
O1 ⁱ —Li1—N7	108.3 (3)	C8—N7—Li1	119.3 (3)
O4—Li1—O3	104.1 (3)	C5—N7—Li1	136.3 (3)
O4—Li1—N7	103.6 (2)		

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

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3—H31 ⁱ ...O4 ⁱ	0.86 (3)	1.98 (3)	2.814 (3)	163 (5)
O3—H32 ⁱ ...N3 ⁱⁱ	0.86 (3)	2.00 (3)	2.820 (4)	159 (5)
O4—H41 ⁱ ...O1 ⁱⁱ	0.87 (3)	1.86 (3)	2.689 (3)	159 (5)
O4—H42 ⁱ ...O2	0.86 (3)	1.86 (3)	2.719 (3)	170 (6)
N1—H1 ⁱ ...O3 ⁱⁱⁱ	0.86	2.13	2.985 (4)	171
N9—H9 ⁱ ...O2 ^{iv}	0.86	1.94	2.760 (3)	158

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

All H atoms were clearly resolved in difference maps. Those bonded to C and N atoms were treated as riding atoms (C—H 0.93 \AA and N—H 0.86 \AA). The O—H distances in the water molecule were controlled by a *SHELXL97 DFIX* command (Sheldrick, 1997), with an overall O—H distance as a free variable (see Table 2 for O—H distances). An overall isotropic vibration parameter for the water H atoms was initially refined as a free variable and in the final cycles was set at the refined value (0.054 \AA^2). No correction was required for extinction. With no atoms having significant anomalous dispersion being present, the few measured Friedel reflections were merged to give the reflection file used in the final refinement.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992a); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* and *PROCESS* (Molecular Structure Corporation, 1992b); program(s) used to solve structure: *SIR88* (Burla *et al.*, 1989) and *DIRDIF* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2000); software used to prepare material for publication: IUCr *SHELXL97* template.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1536). Services for accessing these data are described at the back of the journal.

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