

Table 1. Atom positions ( $\times 10^4$ ) and equivalent isotropic thermal parameters ( $\text{\AA}^2 \times 10^4$ )
$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	$U_{eq}$
Mg	0	3878 (2)	2500	268
C1	-995 (4)	2044 (3)	3886 (2)	286
C2	456 (4)	3034 (3)	4294 (2)	265
C3	1674 (4)	2056 (3)	4844 (2)	254
O11	-1824 (3)	1157 (2)	4316 (2)	378
O12	-1280 (3)	2230 (3)	3130 (1)	370
O2	1346 (3)	3769 (2)	3656 (1)	300
O3	2222 (3)	742 (2)	4421 (1)	314
O10	-1707 (4)	5458 (4)	2853 (2)	550

difference Fourier synthesis showed a maximum value of 0.25 and a minimum value of  $-0.371 \text{ e \AA}^{-3}$ ; atom scattering factors from *International Tables for X-ray Crystallography* (1974).

Fig. 1 shows the anion and numbering scheme and Fig. 2 the packing of the molecules in the unit cell. Table 1\* lists atom parameters; Table 2 gives bond distances and angles. Each  $\text{Mg}^{2+}$  ion bridges two galactarate ions and the coordination of the  $\text{Mg}^{2+}$  ion is octahedral as is normally found (Brown, 1988).

**Related literature.** The galactarate ion has been studied as the  $\text{Ca}^{2+}$  and  $\text{Ba}^{2+}$  salts (Sheldrick, Mackie & Akrigg, 1989), while the coordination of  $\text{Ca}^{2+}$  with the glucarate ion has been established (Burden, Mackie & Sheldrick, 1985; Taga & Osaki, 1976) where the Ca—O distances agree with values given by Dheu-Andries & Perez (1983).

\* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51803 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## Structure of the Sodium Salt of a Thiazolopyrimidine, a Guanine Analog

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**Abstract.** Sodium pentahydrate salt of 2,5-diamino-[1,3]thiazolo[4,5-d]pyrimidin-7(6H)-one,  $[\text{C}_5\text{H}_4\text{N}_5\text{OS}]^- \cdot [\text{Na}(\text{H}_2\text{O})_5]^+$ ,  $M_r = 295.25$ , triclinic,  $P\bar{1}$ ,  $a = 6.9985$  (9),  $b = 8.8182$  (15),  $c = 10.868$  (2)  $\text{\AA}$ ,  $\alpha = 111.83$  (3),  $\beta = 99.83$  (2),  $\gamma = 94.18$  (2) $^\circ$ ,  $V = 606.6$  (2)  $\text{\AA}^3$ ,  $Z = 2$ ,  $D_x = 1.616 \text{ g cm}^{-3}$ ,  $\lambda(\text{Cu K}\alpha) =$

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ) with e.s.d.'s

C1—O11	1.242 (4)	C2—C3	1.529 (4)
C1—O12	1.260 (4)	C3—O3	1.419 (3)
C1—C2	1.535 (4)	C3—C3'	1.547 (5)
C2—O2	1.425 (3)		
O11—C1—O12	124.9 (3)	O2—C2—C3	113.1 (2)
O11—C1—C2	118.8 (3)	C2—C3—O3	110.6 (2)
O12—C1—C2	116.3 (2)	C2—C3—C3'	101.3 (3)
C1—C2—O2	107.0 (2)	O3—C3—C3'	99.3 (3)
C1—C2—C3	110.1 (2)		
Magnesium coordination			
Mg—O12 (O12')	2.050 (2)	Mg—O2(O2')	2.117 (2)
Mg—O10 (O10')	2.003 (3)		
O2—Mg—O12	74.8 (1)	O12—Mg—O12'	90.1 (1)
O10—Mg—O12	90.9 (1)	O10—Mg—O10'	92.3 (2)
O10—Mg—O2	93.8 (1)		

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Table 1. Summary of data collection and structure refinement for (1)

(A) Data collection (295 K)*†	
Mode	$\omega$ -2 $\theta$ scan
Scan range (°)	0.80 + 0.15 tan $\theta$
Background	Scan 0.25 times scan range before and after scan
Scan rate (° min <sup>-1</sup> )	1.4–8.3
Exposure time (h)	17.4
Stability-correction range on I	1.000–1.036
2 $\theta$ range (°)	3.0–152.0
Range in <i>hkl</i> , min.	0, 11, 13
max.	8, 11, 13
Total reflections, measured, unique	2521, 2521
Crystal dimensions (mm)	0.40 × 0.30 × 0.075
Crystal volume (mm <sup>3</sup> )	0.00792
Crystal faces	{010}; {001}; {011}; {201}
Transmission-factor range	0.442–0.805
(B) Structure refinement‡	
Reflections used, <i>m</i> ( $F \geq 4\sigma_F$ )	2411
Number of variables, <i>n</i>	218
Extinction parameter	7.4 (3) × 10 <sup>-6</sup>
Goodness of fit, <i>S</i>	2.352
<i>R</i> , <i>wR</i>	0.0358, 0.0563
<i>R</i> for all data	0.0373
Max., av. $\Delta/\sigma$	0.0099, 0.0008
Max., min. density in $\Delta F$ map (e Å <sup>-3</sup> )	0.49, -0.39

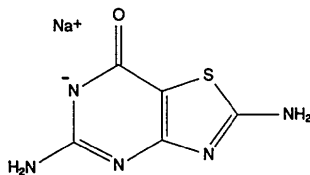
\* Unit-cell parameters were obtained by least-squares refinement of the setting angles of 25 reflections with  $50.2 < 2\theta < 59.6^\circ$ .

† Enraf-Nonius CAD-4 diffractometer with a graphite monochromator was used. Data reduction was accomplished with the SDP-Plus software (Frenz, 1985). Crystal and instrument stability was monitored by remeasurement of 3 check reflections (153; 244; 331) every hour. A linear fit of the intensities of these reflections was used to correct the data.

‡ Function minimized was  $\sum w(F_o - F_c)^2$ , where  $w^{-1} = (\sigma_F^2 + 0.0004F^2)$ .

[1.7397 (15) and 1.751 (2) Å] and the C–S–C angle is 88.53 (8)°. The amino groups are distinct having C–N bond lengths of 1.341 (2) and 1.382 (2) Å. The only interaction between heterocycles is a possible N–H...S hydrogen bond [ $d(\text{N}\cdots\text{S}) = 3.435$  (2) Å;  $d(\text{H}\cdots\text{S}) = 2.82$  (3) Å and  $\angle\text{N–H}\cdots\text{S} = 124.2^\circ$ ]. All other hydrogen bonding involves the Na-ion octahedra which form centrosymmetric pairs having a common edge. The average Na...O distance is 2.44 (8) Å [range: 2.326 (2)–2.585 (11) Å, including both sites of a disordered H<sub>2</sub>O].

**Experimental.** The title compound (1) was synthesized by the procedure outlined by Baker & Chatfield (1969). Yellowish-brown crystals were grown by cooling a hot 10% NaOH solution of the free heterocycle. The data collection and refinement are summarized in Table 1.



(1)

Table 2. Positional and equivalent isotropic thermal parameters (Å<sup>2</sup>) for non-H atoms in (1)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub> <sup>*</sup>
N1	0.8209 (2)	0.50593 (15)	0.63335 (12)	0.0284 (4)
C2	0.8292 (2)	0.6493 (2)	0.62078 (14)	0.0268 (5)
S3	0.74467 (5)	0.64112 (4)	0.45691 (3)	0.0267 (2)
C4	0.6104 (2)	0.3068 (2)	0.27005 (14)	0.0246 (5)
N5	0.5852 (2)	0.14687 (15)	0.25756 (13)	0.0291 (4)
C6	0.6452 (2)	0.1136 (2)	0.3674 (2)	0.0286 (5)
N7	0.7248 (2)	0.2206 (2)	0.49419 (13)	0.0292 (4)
C8	0.7447 (2)	0.3800 (2)	0.50856 (14)	0.0244 (5)
C9	0.6918 (2)	0.4274 (2)	0.40066 (14)	0.0241 (5)
N10	0.8986 (2)	0.7948 (2)	0.72455 (15)	0.0375 (5)
O11	0.5616 (2)	0.34113 (13)	0.16466 (11)	0.0308 (4)
N12	0.6314 (3)	-0.0514 (2)	0.3472 (2)	0.0438 (6)
Na	0.92334 (9)	0.28524 (7)	-0.08879 (6)	0.0318 (2)
OW1	1.0852 (2)	0.50864 (15)	-0.13152 (11)	0.0354 (4)
OW2	0.7007 (2)	0.09834 (14)	-0.04547 (12)	0.0364 (4)
OW3	0.9313 (2)	0.1020 (2)	-0.32029 (13)	0.0395 (5)
OW4	1.1889 (2)	0.1822 (2)	-0.0042 (2)	0.0527 (6)
OW5†	0.6348 (2)	0.3770 (2)	-0.1854 (2)	0.0424 (7)
OW5D†	0.587 (2)	0.3839 (12)	-0.1242 (13)	0.055 (3)

\*  $U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* A_{ij}$ , where  $A_{ij}$  is the dot product of the *i*th and *j*th direct-space unit-cell vectors.

† Populations are 0.829 (7):0.171 (7) OW5:OW5D; thermal parameter for OW5D is *U*, not *U*<sub>eq</sub>.

Table 3. Bond lengths (Å) and bond angles (°) in (1)

1	2	3	1–2	1–2–3
C2	N1	C8	1.320 (2)	109.72 (13)
S3	C2	N10	1.751 (2)	120.43 (14)
S3	C2	N1		115.92 (9)
N10	C2	N1	1.341 (2)	123.6 (2)
C9	S3	C2	1.7397 (15)	88.53 (8)
N5	C4	C9	1.360 (2)	116.90 (15)
C9	C4	O11	1.408 (2)	123.33 (14)
O11	C4	N5	1.288 (2)	119.77 (11)
C6	N5	C4	1.340 (2)	118.65 (11)
N7	C6	N12	1.339 (2)	115.5 (2)
N7	C6	N5		128.00 (14)
N12	C6	N5	1.382 (2)	116.44 (13)
C8	N7	C6	1.349 (2)	113.80 (15)
C9	C8	N1	1.388 (2)	116.13 (13)
C9	C8	N7		122.77 (11)
N1	C8	N7	1.380 (2)	121.10 (15)
S3	C9	C4		130.47 (14)
S3	C9	C8		109.70 (9)
C4	C9	C8		119.83 (14)
OW1	Na	OW2	2.432 (2)	166.94 (5)
OW2	Na	OW3	2.412 (2)	96.98 (5)
OW3	Na	OW4	2.446 (2)	90.27 (6)
OW4	Na	OW5	2.326 (2)	176.66 (6)
OW5	Na	OW1*	2.445 (2)	88.52 (7)
OW1*	Na	OW1	2.423 (2)	86.58 (5)
OW1	Na	OW3		87.80 (5)
OW1	Na	OW4		101.89 (6)
OW1	Na	OW5		80.62 (6)
OW2	Na	OW4		90.27 (6)
OW2	Na	OW5		87.42 (6)
OW2	Na	OW1*		87.89 (5)
OW3	Na	OW5		87.61 (6)
OW3	Na	OW1*		173.63 (5)
OW4	Na	OW1*		93.81 (6)
OW5D	Na	OW1	2.585 (11)	91.7 (3)
OW5D	Na	OW2		75.4 (3)
OW5D	Na	OW3		101.6 (3)
OW5D	Na	OW4		162.3 (3)
OW5D	Na	OW1*		75.6 (3)

\* Denotes equivalent position 2–*x*, 1–*y*, –*z*.

The positions of the Na ion and non-H atoms of the heterocycle were obtained by direct methods (*MULTAN*82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982); the five O atoms of the waters of solvation were located in a difference map. A difference map calculated at  $R = 0.058$  revealed 14 H atoms ( $0.28\text{--}0.66 \text{ e } \text{\AA}^{-3}$ ) and a peak of  $1.15 \text{ e } \text{\AA}^{-3}$  near *OW5* and within coordinating distance to the Na ion. This latter peak was assumed to be a disordered position of *OW5* since it is too close to *OW5* to be present in the same asymmetric unit with *OW5*. The occupancies of the *OW5/OW5D* pair refined to  $0.829(7):0.171(7)$  under the constraint that their sum be 1.00. During the final cycles, all atomic positions, site occupancy of *OW5/OW5D*, anisotropic thermal

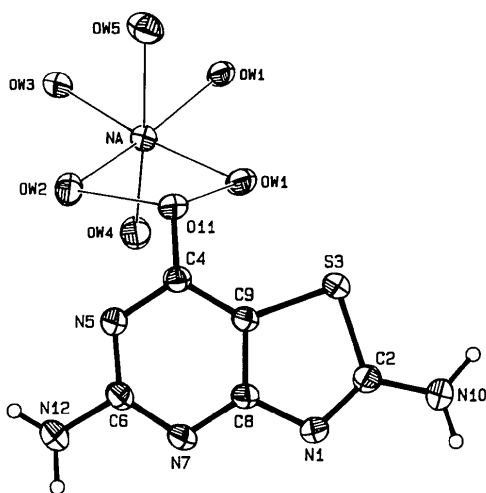


Fig. 1. Perspective drawing of (1) indicating atom labeling. Thermal ellipsoids are drawn at the 50% probability level.

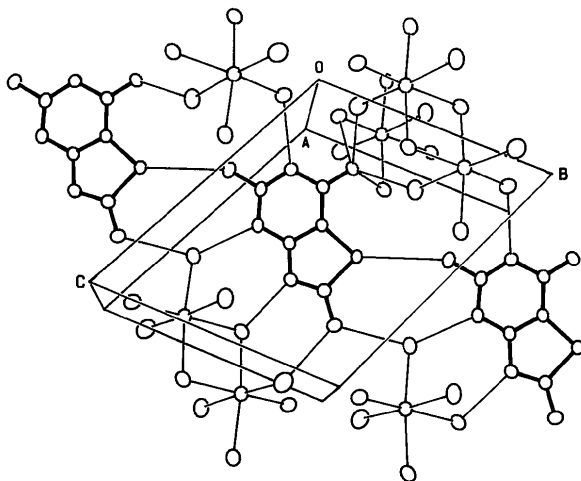


Fig. 2. Perspective drawing of the molecular packing as viewed perpendicular to the plane of the heterocycle. The hydrogen bonding is indicated by thin lines.

Table 4. *Hydrogen bonding in (1)*

<i>D</i> — <i>H</i> ... <i>A</i>	Symmetry of <i>A</i> relative to <i>D</i>	<i>d</i> ( <i>D</i> ... <i>A</i> ) (Å)	<i>d</i> ( <i>H</i> ... <i>A</i> ) (Å)	$\angle$ ( <i>D</i> — <i>H</i> ... <i>A</i> ) (°)
N10 H10A OW4	$2-x, 1-y, 1-z$	3.138 (2)	2.31 (3)	154. (2)
N10 H10B OW3	$x, 1+y, 1+z$	2.926 (2)	2.00 (3)	169. (2)
N12 H12A S3	$x, y-1, z$	3.435 (2)	2.82 (3)	124. (2)
N12 H12B OW5	$1-x, -y, -z$	3.026 (2)	2.33 (3)	139. (2)
N12 H12B OW5D	$1-x, -y, -z$	3.100 (13)	2.33 (3)	149. (3)
OW1 HW1A N1	$x, y, z-1$	2.879 (2)	2.08 (2)	177. (2)
OW1 HW1B O11	$2-x, 1-y, -z$	2.860 (2)	2.10 (2)	160. (3)
OW2 HW2A O11	$x, y, z$	2.859 (2)	2.09 (2)	162. (2)
OW2 HW2B N5	$1-x, -y, -z$	2.843 (2)	2.06 (2)	168. (2)
OW3 HW3A N7	$x, y, z-1$	2.836 (2)	2.05 (3)	172. (2)
OW3 HW3B N12	$2-x, -y, -z$	3.172 (2)	2.404 (14)	163. (3)
OW4 HW4A O11	$1+x, y, z$	2.839 (2)	2.04 (2)	175. (2)
OW4 HW4B OW2	$2-x, -y, -z$	2.853 (2)	2.122 (15)	153. (5)
OW5 HW5A O11	$1-x, 1-y, -z$	2.882 (2)	2.09 (2)	174. (3)
OW5D HW5A O11	$1-x, 1-y, -z$	2.856 (11)	2.09 (2)	135. (2)

parameters for non-H atoms and isotropic thermal parameters for H atoms were varied except that *OW5D* was refined isotropically, the H atoms of the water molecules were given a single isotropic thermal parameter which was refined, and the waters were constrained to have the same geometry [*i.e.* all  $d(\text{O—H})$  and  $d(\text{H}\cdots\text{H})$  were equivalent but varied]. No H atoms were found for *OW5D*, but *HW5A* is within bonding distance and therefore *HW5A* was given full occupancy while the occupancy of *HW5B* was equated to that of *OW5*. A full-matrix least-squares refinement was used (*SHELX76*; Sheldrick, 1976). Scattering factors and anomalous-dispersion corrections were taken from *International Tables for X-ray Crystallography* (1974) except those for H which were taken from Stewart, Davidson & Simpson (1965). Data were reduced with *SDP-Plus* (Frenz, 1985); least-squares planes calculated with program *PLANES* from Cordes (1983); thermal-ellipsoid plots produced with *ORTEPII* (Johnson, 1976). Parameter, geometry and structure-factor-amplitude tables were prepared with programs *FUER* and *LISTFC* (Larson, 1980).

Atomic coordinates are listed in Table 2;\* Na coordination, bond lengths and bond angles are given in Table 3. Fig. 1 is a perspective drawing of the molecule illustrating atom labeling; Fig. 2 illustrates the intermolecular hydrogen bonding which is numerically detailed in Table 4.

**Related literature.** No thiazolopyrimidine structures have been reported (Cambridge Structural Database, 1987).

\* Tables of anisotropic thermal parameters, H-atom parameters, bond lengths and angles involving H atoms, torsion angles, least-squares planes and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51622 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## Structure of Chloro(3,7-diazanonanediamide)nickel(II) Perchlorate

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**Abstract.**  $[\text{NiCl}(\text{C}_7\text{H}_{16}\text{N}_4\text{O}_2)]\text{ClO}_4$ ,  $M_r = 381.8$ , triclinic,  $P\bar{1}$ ,  $a = 7.822$  (3),  $b = 7.924$  (3),  $c = 12.637$  (4) Å,  $\alpha = 107.37$  (3),  $\beta = 91.52$  (3),  $\gamma = 110.50$  (3)°,  $V = 692.6$  (5) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 1.831$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 18.2$  cm<sup>-1</sup>,  $F(000) = 392$ ,  $T = 296$  K,  $R = 4.37\%$ ,  $wR = 4.79\%$  for 2189 independent reflections with  $I > 3.0\sigma(I)$ . This compound is a five-coordinate Ni complex. The nickel(II) ion is in a slightly distorted square pyramid with the diaminodiamide equatorial and a Cl anion axial.

**Experimental.** The ligand, *L*-1,3,1, was prepared from 1,3-propanediamine (41.5 ml, 0.5 mol) and 2-chloroacetamide (55.8 g, 0.6 mol) in *N,N'*-dimethylformamide (50 ml) by heating under reflux for 2 h. The title compound was obtained by adding *L*-1,3,1 (5.26 g) to an aqueous solution of nickel(II) perchlorate (4.76 g) and heating until it was completely dissolved; the solution was filtered immediately while hot. After evaporation of the filtrate, deep-blue rod-like crystals of  $[\text{NiCl}(\text{L}-1,3,1)]\text{ClO}_4$  were formed. A crystal  $0.22 \times 0.28 \times 0.40$  mm was selected for the determination of lattice constants (18 reflections,  $11.0 \leq 2\theta \leq 27.4^\circ$ , Mo *K*α radiation, Nicolet *R2m/V* diffractometer, graphite monochromator) as well as for the data collection. Corrections for absorption effects were based on  $\psi$  scans of a few suitable reflections with  $\chi$  values close to  $90^\circ$ . Max./min. transmission factors: 0.925/0.622. Total of 3007 reflections measured with  $[(\sin\theta)/\lambda]_{\text{max}} = 0.595$  Å<sup>-1</sup> and in the range  $0 \leq h \leq 9$ ,

$-9 \leq k \leq 8$ ,  $-15 \leq l \leq 15$ . No significant variation in intensities of three standards monitored every 50 reflections. Scan width of  $1.2^\circ$  plus *K*α separation and scan speed  $2.93\text{--}14.65^\circ$  min<sup>-1</sup>. 2189 unique structure amplitudes with  $I > 3.0\sigma(I)$ . The structure was solved by direct methods and refined by full-matrix least squares based on *F* values. All of the non-H atoms were refined anisotropically. H atoms were placed in idealized positions (C–H = 0.96 Å, H–C–H =  $109.4^\circ$ ) and refined with fixed *U* (0.08 Å<sup>2</sup>). At convergence  $R = 4.37\%$ ,  $wR = 4.79\%$ ,  $w = [\sigma^2(F) + 0.00068F^2]^{-1}$ ,  $\sigma^2(F)$  based on counting statistics,

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement coefficients (Å<sup>2</sup>  $\times 10^3$ )

Equivalent isotropic *U* defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub>
Ni	2058 (1)	4438 (1)	1866 (1)	26 (1)
O(1)	1708 (3)	2054 (3)	669 (2)	34 (1)
O(2)	-234 (3)	4545 (3)	1269 (2)	37 (1)
N(1)	1907 (4)	6437 (4)	3223 (2)	31 (1)
N(2)	3860 (4)	3763 (4)	2646 (2)	32 (1)
N(3)	2495 (5)	-495 (5)	282 (3)	44 (1)
N(4)	-1607 (4)	6609 (5)	1348 (3)	38 (1)
C(1)	2743 (4)	1249 (4)	857 (3)	31 (1)
C(2)	4384 (5)	2397 (5)	1774 (3)	37 (1)
C(3)	5433 (5)	5461 (5)	3376 (3)	33 (1)
C(4)	4778 (5)	6715 (5)	4282 (3)	34 (1)
C(5)	3737 (5)	7762 (5)	3906 (3)	34 (1)
C(6)	903 (5)	7448 (5)	2825 (3)	37 (1)
C(7)	-389 (4)	6106 (5)	1749 (3)	29 (1)
Cl(1)	4198 (1)	6812 (1)	1027 (1)	36 (1)
Cl(2)	-761 (1)	1672 (1)	3595 (1)	42 (1)
O(4)	-331 (7)	1048 (6)	2507 (4)	90 (2)
O(5)	-1784 (5)	65 (5)	3884 (4)	86 (2)
O(6)	-1702 (9)	2888 (8)	3663 (6)	131 (4)
O(7)	936 (8)	2694 (9)	4287 (4)	140 (3)

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