C6—N7	1.312 (3)	C6P—N7P	1.309 (3)
N7—C8	1.369 (3)	N7P—C8P	1.375 (3)
C8—C8A	1.369 (3)	C8P—C8AP	1.371 (3)
C8—C81	1.476 (3)	C8P—C81P	1.481 (3)
C81—O83	1.193 (3)	C81P—O83P	1.197 (3)
C81—O82	1.321 (3)	C81P—O82P	1.317 (3)
C31—C32	1.501 (4)	C31P—C32P	1.492 (4)
C32—Cl1	1.790 (3)	C32P—Cl1P	1.782 (3)

C8A—C8—C81—O82	177.5 (2)
N3—C31—C32—Cl1	64.9 (2)
C8AP—C8P—C81P—O82P	−174.0 (2)
N3P—C31P—C32P—Cl1P	73.9 (3)

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H···A		D···A
O82—H82···N7P		2.879 (3)
C6P—H6P···O83		2.938 (3)
O82P—H82P···N7$^{\text{i}}$		2.753 (3)
C6—H6···O83P$^{\text{i}}$		3.191 (3)

Symmetry code: (i) $1 - x, 2 - y, 1 - z$.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *DATRED* (Brookhaven National Laboratory & Birmingham University, 1986). Program(s) used to solve structure: *MULTAN*80 (Main *et al.*, 1980). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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Heptahydrated Monosodium Salt of 6-Amino-5-(2-carboxyphenyl)azouracil

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Abstract

The bulky organic molecule in the title compound, sodium 2-[6-amino-2,4(3H,5H)-dioxopyrimidin-5-ylazo]benzoate heptahydrate, $Na^+.C_{11}H_8N_5O_4^-.7H_2O$, exists as a monovalent anion with negatively charged carboxylate and uracil groups and a protonated azo group. An intramolecular bifurcated hydrogen bond contributes to the approximate planarity of the anion.

Comment

The dinuclear copper(II) complex [Cu(μ-HL^1)Cu(H$_2$O)$_2$-(CH$_3$CH$_2$OH)](ClO$_4$)$_3$ [H$_2L^1$ = α,ω-bis(1,3-dimethyl-5-nitrosouracil-6-ylamino)propane], which contains *syn–syn* oximato bridging groups, has been found to form mixed-bridged trinuclear complexes such as [(μ-L){Cu(μ-L)Cu(H$_2$O)Cu(μ-L)}](ClO$_4$)$_2$.4.88H$_2$O (Colacio, Dominguez-Vera, Escuer, Klinga, Kivekäs & Romerosa, 1995). In an attempt to obtain an analogous trinuclear complex containing a hydroxide ion instead of the chloride bridging ion, we obtained, surprisingly, a hydrated monosodium salt of 6-amino-5-(2-carboxyphenyl)azouracil (H$_2L$). We have recently prepared other non-coordinated phenylazouracil derivatives: the cations 6-amino-1,3-dimethyl-5-(phenylazonio)uracil (Kivekäs, Colacio, Ruiz, López-González & León, 1989), 6-amino-1,3-dimethyl-5-(2-ethylphenylazonio)uracil (Kivekäs, Sundberg, Ruiz & Colacio, 1991; Kivekäs, Ruiz & Colacio, 1994) and 6-amino-1,3-dimethyl-5-(2-carboxyphenylazonio)uracil (Sundberg, Kivekäs, Ruiz, Moreno & Colacio, 1992). In these structures, the bulky non-coordinated molecules exist as monovalent cations, the N8 atom of the azo group being protonated. In the metal complexes, the phenylazouracil and analogous barbituric acid derivatives coordinate as anionic ligands and the N8 atom of the neutral azo group is coordinated to the metal (Colacio, Dominguez-Vera, Kivekäs, Moreno &

Ruiz, 1994). Now, for the first time, we have obtained an anionic non-coordinated 2-phenylazouracil derivative in which the N8 atom is protonated, and report here the preparation of this derivative, (I), and its crystal structure.

(I)
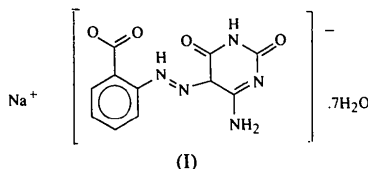
The structure of $Na^+.C_{11}H_8N_5O_4^-.7H_2O$ is formally ionic, containing bulky organic anions (HL^-), Na^+ ions and crystal water molecules, connected by an extensive hydrogen-bonding network. However, as the Na^+ ions are connected by bridges formed by the water-molecule O atoms, the structure may be better described as polymeric, containing infinite $[Na(H_2O)_4]_n^{n+}$ chains, bulky HL^- counterions and lattice water molecules linked by hydrogen bonds.

The non-coordinated H_2L molecule can exist in several different forms in the solid state, as H_2L has several possible atoms or atom groups that can influence the charge of the molecule and the substituted uracil group can assume different tautomeric forms. In the title compound, the carboxylate group of the HL^- ion is in the anionic form and the azo group is protonated. The negative charge of the substituted uracil ring results in an overall negative charge for HL^-, which is necessary to balance the charges of the salt.

Despite the negative charge, the characteristic features reported for non-coordinated positively charged 2-substituted phenylazouracil derivatives are also observed for HL^-; the carboxylate substituent is on the same side of the molecule as the N8—H8 bond, the molecule is approximately planar, and H8 participates in an intramolecular hydrogen bond. However, comparison of the bond lengths in the title compound and those found for the other 1,3-dimethyl substituted uracil derivatives, except those for which the study was of very low accuracy (Kivekäs, Ruiz & Colacio, 1994), reveals slight differences. In the title compound, the bonds to N1 seem to be *ca* 0.04 Å shorter than in the other compounds. Even though the differences are not all significant, there is a clear trend indicating an increase in the double-bond character of the N1—C2 and N1—C6 bonds. The C—O distances in the uracil group [1.250 (7) and 1.240 (7) Å] are slightly longer than in the 1,3-dimethyl substituted uracil derivatives, but are still closer to C=O than to C—OH bond distances, indicating a double bond between the atoms. Moreover, no electron density typical of an H atom was found in the vicinity of the O atoms O2 or O4. A difference Fourier map also clearly indicated that an H atom is attached to the N3 atom, but not to N1, and that the carboxylate group is deprotonated.

The hydrogen-bonding scheme confirms this atomic arrangement.

The protonation takes place at the azo N8 atom and the H atom is in a favorable position to form a bifurcated intramolecular hydrogen bond to the O atoms O4 and O16. A similar bifurcated hydrogen bond was found in the analogous 6-amino-1,3-dimethyl-5-(2-carboxyphenylazonio)uracil cation (Sundberg, Kivekäs, Ruiz, Moreno & Colacio, 1992). An intramolecular hydrogen bond between N8 and O4 has been reported for the analogous 6-amino-1,3-dimethyl-5-(phenylazonio)uracil cation (Kivekäs, Colacio, Ruiz, López-González & León, 1989) and the 6-amino-1,3-dimethyl-5-(2-ethylphenylazonio)uracil cation (Kivekäs, Sundberg, Ruiz & Colacio, 1991; Kivekäs, Ruiz & Colacio, 1994). The planarity of these bulky organic molecules is enhanced by the strong intramolecular hydrogen bond (Kivekäs, Sundberg, Ruiz & Colacio, 1991).

Six O atoms of lattice water molecules surround each Na^+ ion with Na—O distances in the range 2.372 (5)–2.497 (5) Å, forming a distorted octahedral coordination sphere around the cation. In each NaO_6 coordination sphere, four of the O atoms bridge pairs of Na^+ ions, forming a polymeric $[Na(H_2O)_4]_n^{n+}$ chain.

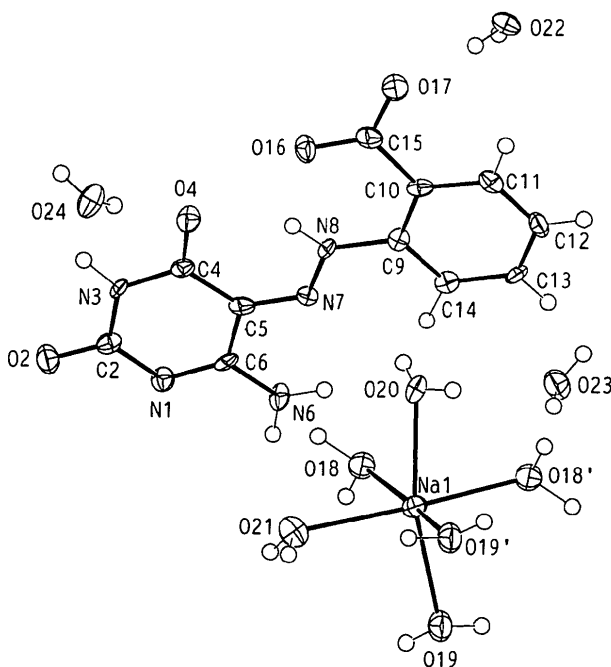Fig. 1. *ORTEP* plot of the title compound showing the numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as small circles of arbitrary radii.

Experimental

The title compound was obtained by adding solid Na_2CO_3 (0.5 mmol) to a stirred suspension of $[Cu(\mu\text{-}HL)Cu(H_2O)_2\text{-}(CH_3CH_2OH)](ClO_4)_3$ (1 mmol) [prepared as reported by

Colacio *et al.* (1995)] in an ethanol/water mixture (5:1). After 15 min a clear orange solution was obtained, which, kept at ambient temperature, yielded orange crystals. These were collected by filtration and air dried.

Crystal data

$Na^+.C_{11}H_8N_5O_4^-.7H_2O$	Mo $K\alpha$ radiation
$M_r = 423.33$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 25
$P2_1/c$	reflections
$a = 6.646\,(3)$ Å	$\theta = 20$–$25°$
$b = 20.599\,(6)$ Å	$\mu = 0.15$ mm^{-1}
$c = 13.458\,(5)$ Å	$T = 213\,(2)$ K
$\beta = 90.61\,(5)°$	Plate
$V = 1842\,(1)$ Å^3	$0.40 \times 0.30 \times 0.25$ mm
$Z = 4$	Orange
$D_x = 1.526$ Mg m^{-3}	

Data collection

Rigaku AFC-7S diffractom-	$R_{int} = 0.034$
eter	$\theta_{max} = 24.99°$
$2\theta/\omega$ scans	$h = 0 \rightarrow 7$
Absorption correction:	$k = 0 \rightarrow 24$
empirical *via* ψ scans	$l = -15 \rightarrow 16$
$T_{min} = 0.938$, $T_{max} =$	3 standard reflections
1.00	monitored every 200
3228 measured reflections	reflections
1885 independent reflections	intensity decay: 1%
1885 observed reflections	
$[F > 4.0\sigma(F)]$	

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.27$
$R = 0.081$	$\Delta\rho_{max} = 0.56$ e Å^{-3}
$wR = 0.061$	$\Delta\rho_{min} = -0.466$ e Å^{-3}
$S = 1.421$	Extinction correction: none
1885 reflections	Atomic scattering factors
320 parameters	from *International Tables*
Only coordinates of H atoms	*for X-ray Crystallography*
refined	(1974, Vol. IV, Tables
Weighting scheme based	2.2B and 2.3.1)
on measured e.s.d.'s	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Na1	0.7469 (4)	0.4810 (1)	0.9506 (2)	0.023 (1)
N1	0.2737 (8)	0.6882 (2)	0.3903 (4)	0.021 (3)
O2	0.2877 (7)	0.7817 (2)	0.4765 (3)	0.029 (3)
C2	0.2839 (9)	0.7210 (3)	0.4765 (4)	0.019 (4)
N3	0.2943 (7)	0.6897 (2)	0.5667 (3)	0.017 (3)
O4	0.2820 (7)	0.5983 (2)	0.6608 (3)	0.025 (3)
C4	0.2812 (9)	0.6239 (3)	0.5774 (4)	0.018 (4)
C5	0.2692 (9)	0.5868 (3)	0.4854 (4)	0.018 (3)
N6	0.2586 (8)	0.5916 (2)	0.3084 (3)	0.021 (3)
C6	0.2670 (8)	0.6240 (3)	0.3930 (4)	0.017 (4)
N7	0.2552 (7)	0.5238 (2)	0.4773 (3)	0.015 (3)
N8	0.2507 (7)	0.4861 (2)	0.5546 (3)	0.017 (3)
C9	0.2343 (8)	0.4179 (3)	0.5424 (4)	0.016 (3)
C10	0.2286 (9)	0.3769 (3)	0.6248 (4)	0.019 (4)
C11	0.2119 (9)	0.3101 (3)	0.6076 (4)	0.019 (4)
C12	0.2008 (9)	0.2851 (3)	0.5132 (5)	0.024 (4)
C13	0.2075 (9)	0.3263 (3)	0.4333 (4)	0.021 (4)
C14	0.2268 (9)	0.3926 (3)	0.4451 (4)	0.019 (4)

C15	0.2451 (9)	0.4020 (3)	0.7310 (5)	0.023 (4)
O16	0.2373 (6)	0.4620 (2)	0.7454 (3)	0.024 (3)
O17	0.2610 (7)	0.3600 (2)	0.7998 (3)	0.027 (3)
O18	0.4245 (7)	0.4220 (2)	0.9787 (3)	0.029 (3)
O19	0.9341 (7)	0.4714 (2)	1.1009 (3)	0.030 (3)
O20	0.6114 (7)	0.5195 (2)	0.7953 (3)	0.031 (3)
O21	0.8651 (7)	0.3752 (2)	0.8913 (3)	0.029 (3)
O22	0.5422 (6)	0.2552 (2)	0.7711 (3)	0.024 (3)
O23	0.6602 (7)	0.6502 (2)	0.8364 (3)	0.033 (3)
O24	0.0783 (7)	0.6573 (2)	0.8209 (3)	0.034 (3)

Table 2. *Selected geometric parameters* (Å, °)

Na1—O18	2.497 (5)	N3—C4	1.367 (8)
Na1—O19	2.372 (5)	O4—C4	1.240 (7)
Na1—O20	2.401 (5)	C4—C5	1.456 (8)
Na1—O21	2.453 (5)	C5—C6	1.461 (8)
Na1—O18^i	2.494 (5)	C5—N7	1.306 (8)
Na1—O19^{ii}	2.442 (5)	N6—C6	1.320 (8)
N1—C2	1.343 (8)	N7—N8	1.299 (7)
N1—C6	1.323 (8)	N8—C9	1.418 (8)
O2—C2	1.250 (7)	C15—O16	1.251 (8)
C2—N3	1.375 (8)	C15—O17	1.270 (8)
O18—Na1—O19	105.9 (2)	N3—C4—C5	115.7 (5)
O18—Na1—O20	88.7 (2)	O4—C4—C5	123.1 (6)
O18—Na1—O21	83.9 (2)	C4—C5—C6	116.7 (5)
O18—Na1—O18^i	86.4 (2)	C4—C5—N7	126.5 (5)
O19—Na1—O21	92.1 (2)	C6—C5—N7	116.8 (5)
O19—Na1—O18^i	88.8 (2)	N1—C6—C5	123.2 (5)
O19—Na1—O19^{ii}	80.0 (2)	N1—C6—N6	118.9 (5)
O20—Na1—O21	97.4 (2)	C5—C6—N6	117.9 (5)
O20—Na1—O18^i	84.2 (2)	C5—N7—N8	121.9 (5)
O20—Na1—O19^{ii}	86.5 (2)	N7—N8—C9	120.1 (5)
O21—Na1—O19^{ii}	89.0 (2)	N8—C9—C10	120.7 (5)
O18^i—Na1—O19^{ii}	100.9 (2)	N8—C9—C14	118.4 (5)
C2—N1—C6	118.8 (5)	C9—C10—C15	122.5 (6)
N1—C2—O2	120.3 (5)	C11—C10—C15	119.6 (5)
N1—C2—N3	121.8 (5)	C10—C15—O16	118.6 (5)
O2—C2—N3	117.9 (5)	C10—C15—O17	117.2 (6)
C2—N3—C4	123.8 (5)	O16—C15—O17	124.3 (6)
N3—C4—O4	121.2 (5)		

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

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$\cdots$O22^i	0.91 (5)	1.90 (5)	2.778 (6)	159 (5)
N6—H6A$\cdots$O21^{ii}	0.94 (5)	2.03 (5)	2.885 (5)	151 (5)
N6—H6B$\cdots$O20^{ii}	0.89 (5)	2.12 (5)	2.821 (7)	135 (4)
N8—H8$\cdots$O4	0.89 (5)	2.02 (5)	2.742 (6)	136 (4)
N8—H8$\cdots$O16	0.89 (5)	2.00 (5)	2.618 (6)	125 (4)
O18—H18A$\cdots$O17	1.02 (5)	1.93 (5)	2.924 (6)	162 (5)
O18—H18B$\cdots$O23^{iii}	0.80 (5)	2.22 (5)	2.957 (6)	155 (5)
O19—H19A$\cdots$O16^{iii}	1.00 (6)	1.76 (5)	2.740 (6)	164 (5)
O19—H19B$\cdots$O24^{iii}	0.78 (6)	2.09 (6)	2.854 (7)	165 (5)
O20—H20A$\cdots$O23	0.73 (6)	2.04 (6)	2.767 (6)	173 (6)
O20—H20B$\cdots$O16	0.71 (6)	2.13 (6)	2.829 (6)	168 (6)
O21—H21A$\cdots$O2^{iv}	0.89 (4)	1.94 (4)	2.819 (6)	171 (4)
O21—H21B$\cdots$O17^v	0.84 (5)	2.13 (5)	2.935 (6)	159 (5)
O22—H22A$\cdots$O17	0.84 (5)	2.05 (5)	2.884 (6)	171 (4)
O22—H22B$\cdots$N1^{ii}	1.01 (5)	1.79 (5)	2.763 (6)	161 (4)
O23—H23A$\cdots$O24^v	0.82 (6)	1.98 (6)	2.793 (7)	169 (6)
O23—H23B$\cdots$O22^i	0.78 (6)	2.17 (6)	2.922 (6)	163 (5)
O24—H24A$\cdots$O4	0.79 (6)	2.05 (6)	2.830 (6)	170 (6)
O24—H24B$\cdots$O2^{vi}	0.77 (6)	2.03 (6)	2.801 (6)	172 (6)

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993a). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1993b). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *Xtal CRYLSQ*

(Hall, Flack & Stewart, 1992). Molecular graphics: *Xtal ORTEP*. Software used to prepare material for publication: *Xtal BONDLA CIFIO*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, bond distances and angles involving H atoms, least-squares-planes data and torsion angles have been deposited with the IUCr (Reference: HU1133). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A 1,2-Dihydrodipyrido[1,2-b:3',2'-d]-pyrazol-2-one

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Abstract

The pyrazole and pyridine rings in the pyrazolo[1,5-a]-pyridine skeleton of 1-ethyl-2-oxo-1,2-dihydrodipyrido-[1,2-b:3',2'-d]pyrazole-3-carbonitrile, C$_{13}$H$_{10}$N$_4$O, are planar [maximum deviations 0.004 (3) and 0.004 (3) Å, respectively], and are almost coplanar to each other with

a dihedral angle of 0.9 (3)°. The planar 2-pyridone ring (fused to the pyrazolo[1,5-a]pyridine ring at the 2- and 3-positions) is also nearly coplanar with the pyrazolo[1,5-a]pyridine ring [maximum deviation 0.032 (3) Å, dihedral angle 0.9 (3)°]. The delocalized ring system extends to the fused 2-pyridone ring.

Comment

The present study has been undertaken to confirm the chemical structure of the title compound, (2), and to compare the structural features of some nitrogen-bridged heterocycles such as pyrazolo[1,5-a]pyridines and fused pyrazolo[1,5-a]pyridine derivatives of physicochemical and pharmaceutical interest.
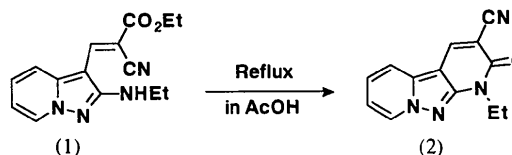
The title molecule is almost planar, except for the terminal C atom of the 1-ethyl group. The bond distances and angles for the pyrazolo[1,5-a]pyridine skeleton in the title compound are very similar to those in the geometry of 3-(p-chlorobenzoylthio)-2-(methylthio)pyrazolo[1,5-a]pyridine (Kakehi, Kitajima, Ito & Takusagawa, 1994) and 2-acetyl-3-amino-5-ethyl-thieno[2',3':3,4]pyrazolo[1,5-a]pyridine (Kakehi *et al.*, 1990). This indicates that the annelation of a six- or five-membered ring at the 2- and 3-positions of the pyrazolo[1,5-a]pyridine moiety does not result in a large difference in the bond distances and angles of the skeleton. On the other hand, the geometry of the attached pyridone ring, especially the lengthened N(1)—C(10) and C(2)—C(3) bonds, is somewhat different from that of the α-pyridone (Penfold, 1953), suggesting that the pyridone moiety in (2) has a different resonance structure from pyridone itself. This is a result of the fused pyrazolo[1,5-a]pyridine ring changing the resonance system of the pyridone ring.

The bond lengths and angles of the pyridine ring in the pyrazolo[1,5-a]pyridine moiety are similar to those in the indolizine derivatives, having no large distortions resulting from the annelation (Kakehi, Kitajima, Ito & Takusagawa, 1993a,b). The bond lengths and angles of the pyrazole ring in the pyrazolo[1,5-a]pyridine moiety are also similar to those of the parent pyrazole (Ehrlich, 1960), except for the lengthened C(4)—C(5) bond, indicating that the pyrazole moiety of the title compound (2) also has a different resonance structure from pyrazole itself. There are no marked differences between the double and single bond lengths within the ring C atoms except for the C(1)—C(2) bond, showing the full extension of aromatic resonance over the ring system.