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Guaninium sulfate monohydrate

Aouatef Cherouana, Nourredine Benali-Cherif* and Lamia Bendjeddou

Laboratoire de Chimie Moléculaire, du Contrôle de l'Environnement et des Mesures Physico-Chimiques, Faculté des Sciences, Département de Chimie, Université Mentouri de Constantine, 25000 Constantine, Algeria

Correspondence e-mail: benalicherif@hotmail.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.081
Data-to-parameter ratio = 11.3

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

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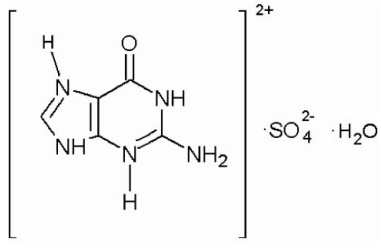
In the crystal structure of the title compound, $C_5H_7N_5O^{2+}\cdot SO_4^{2-}\cdot H_2O$, the guaninium cation, the sulfate anion and the water molecule form a network of hydrogen bonds. The structure consists of layers of guaninium ions and water molecules parallel to the diagonal of the *ac* plane, linked by strong hydrogen bonds.

Comment

The structure elucidation of nucleic acids and their derivatives is of interest, because of their widespread biological occurrence (Richards *et al.*, 1972; Perutz & Eyck, 1972). A number of these compounds are effective metabolic inhibitors with useful chemotherapeutic activity (Roy-Burman, 1970; Balis, 1968; Hitchings & Elion, 1963). In several crystal structures of compounds with organic bases and inorganic acids, the structural cohesion is assured by strong hydrogen bonds, as was observed in guaninium dinitrate dihydrate (Bouchouit *et al.*, 2002), adeninium sulfate (Langer & Huml, 1978*a*), adeninium hemisulfate hydrate (Langer & Huml, 1978*b*) and adeninium hydrobromide hemihydrate (Langer & Huml, 1978*c*). Two structures of guanine with inorganic acids have been reported, namely guaninium dinitrate dihydrate and guaninium dichloride (Matković-Čalogović & Sanković, 1999).



(I)

The determination of the crystal and molecular structure of guaninium sulfate hydrate, (I), forms part of a study of the interactions between organic bases and inorganic acids. The dimensions of the sulfate anion (Fig. 1) are comparable with those found in other sulfates (*e.g.* Cherouana *et al.*, 2002; Srinivasan *et al.*, 2001). The S—O bond lengths are in the range 1.4653 (16)–1.4874 (13) Å, while the O—S—O angles range from 108.23 (8) to 110.88 (9)°. As was observed in guaninium dinitrate dihydrate, the imino groups of the pyrimidine and imidazolyl moieties (N3 and N7) in guanine are protonated. There is an intricate hydrogen-bond network (Fig. 2). The diprotonated guanine in (I) is hydrogen bonded

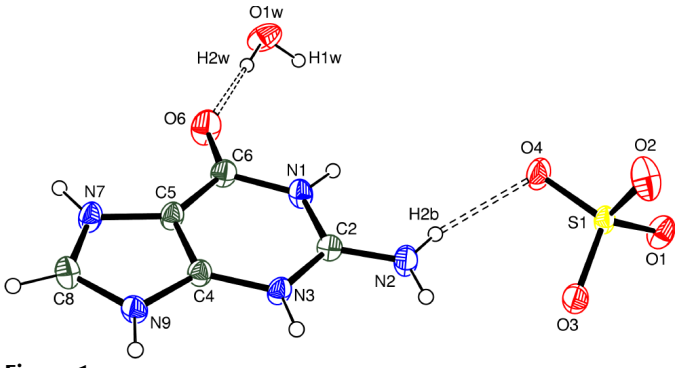


Figure 1
ORTEP-3 (Farrugia, 1997) view of the title compound, with the atomic labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

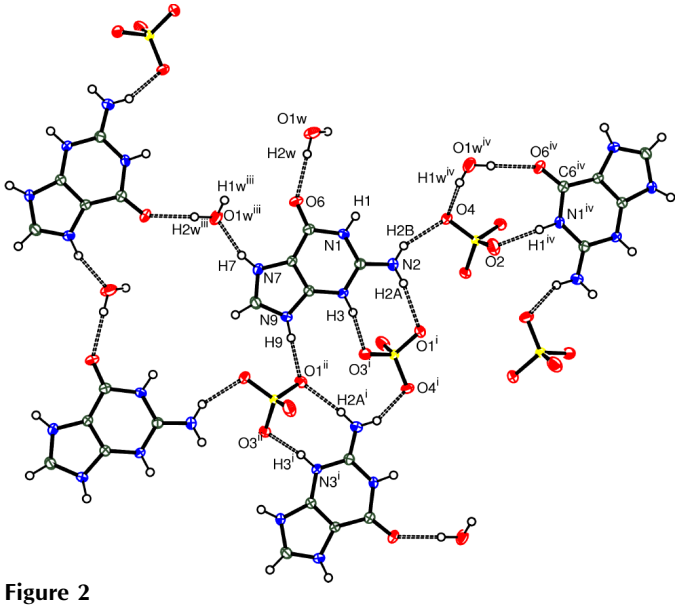


Figure 2
ORTEP-3 (Farrugia, 1997) view, showing the intricate hydrogen-bond interactions between anions and cations. [Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, y+1, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.]

to four sulfate groups [*via* N1—H1···O2 for the first group, N3—H3···O3 and N2—H21···O1 for the second group, N9—H9···O1 for the third and N2—H21···O3 and N2—H22···O4 for the last group]. We also observed that the water molecule forms three hydrogen bonds with the guaninium and sulfate ions, in two modes, *viz*. as donor with the sulfate anion [*via* O1*W*—H1*W*···O4 and O1*W*—H2*W*···O6] and as acceptor with the guaninium ion [*via* N7—H7···O1*W*]. This system of hydrogen bonds among the guaninium cations, the sulfate anions and the water molecule generates a succession of layers parallel to the diagonal of the *ac* plane (Fig. 3). Layers of guaninium cations and water molecules are linked by strong anion–cation and anion–water hydrogen bonds *via* the sandwiched sulfates.

Experimental

Colorless single crystals of guaninium sulfate monohydrate were obtained after two weeks by slow evaporation, at room temperature, of an equimolar aqueous solution of guanine and sulfuric acid.

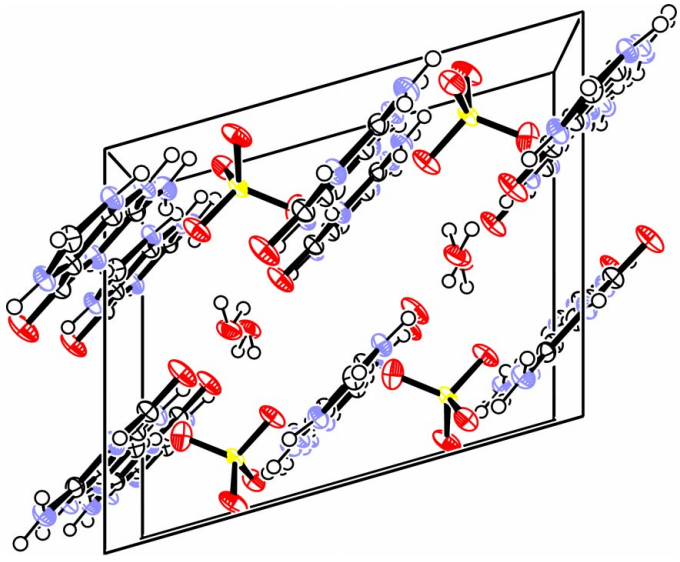


Figure 3
ORTEP-3 (Farrugia, 1997) diagram of the layered packing of the title compound, viewed down the *b* axis.

Crystal data

$C_5H_7N_5O^{2+}\cdot SO_4^{2-}\cdot H_2O$	$D_x = 1.823$ Mg m^{-3}
$M_r = 267.24$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6875 reflections
$a = 8.9940$ (3) Å	$\theta = 2.8$–$26.4°$
$b = 10.2020$ (2) Å	$\mu = 0.37$ mm^{-1}
$c = 11.0440$ (3) Å	$T = 293$ (2) K
$\beta = 106.04$ (2)°	Plate, colorless
$V = 973.9$ (1) Å^3	0.40 × 0.10 × 0.01 mm
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.033$
φ scans	$\theta_{max} = 26.4°$
Absorption correction: none	$h = -11 \rightarrow 11$
6875 measured reflections	$k = -12 \rightarrow 12$
1821 independent reflections	$l = -12 \rightarrow 12$
1631 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.4753P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.032$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.081$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.41$ e Å^{-3}
1821 reflections	
161 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O3^{i}	0.86	1.75	2.6011 (19)	167
N9—H9···O1^{ii}	0.86	1.81	2.6526 (19)	167
N7—H7···O1W^{iii}	0.86	1.80	2.637 (2)	164
N1—H1···O2^{iv}	0.86	1.91	2.738 (2)	160
N2—H2A···O1^{i}	0.86	2.09	2.934 (2)	166
N2—H2B···O4	0.86	2.07	2.829 (2)	146
O1W—H1W···O4^{iv}	0.86 (2)	2.00 (2)	2.838 (2)	164 (3)
O1W—H2W···O6	0.86 (2)	1.93 (2)	2.793 (2)	178 (1)

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

H atoms attached to C and N atoms were fixed at localized positions and refined using a riding model. H atoms belonging to the water molecule were refined with an overall isotropic displacement parameter, using restraints.

Data collection: *KappaCCD Reference Manual* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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