Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Guaninium dihydrogenphosphite dihydrate

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Received 21 July 2003
Accepted 7 August 2003
Online 30 August 2003

The structure of the title compound, $C_5H_6N_5O^+\cdot H_2PO_3^-\cdot 2H_2O$, consists of a layer arrangement in which the organic cations are sandwiched between $H_2PO_3^-$ inorganic sheets. In the crystal structure, the phosphite anions are linked together by short strong (P—O—H···O—P) hydrogen bonds to form a two-dimensional network. Strong hydrogen bonds are responsible for the cohesion between organic–inorganic layers and maintain the stability of the structure.

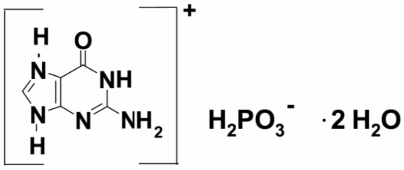
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.082
Data-to-parameter ratio = 11.6

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

Comment

The crystal structures of organic–inorganic hybrid materials have been investigated over the past few decades (Bagieu-Beucher, 1990; Ravikumar *et al.*, 2002). As part of our continuing interest in this field, we report here the crystal structure of guaninium dihydrogenphosphite dihydrate, (I).



(I)

The asymmetric unit contains one guaninium cation, one monohydrogenphosphite anion and two water molecules (Fig. 1). The main feature of the alkyl or aryl ammonium monohydrogenphosphite is that the anionic subnetwork is built up through short strong hydrogen bonds (Blessing, 1986) and the organic cations are bonded to the phosphite layers by weaker hydrogen bonds (Masse & Levy, 1991). The inorganic moiety is a network of $H_2PO_3^-$ tetrahedra, connected by short and strong hydrogen bonds. Inside these chains each $H_2PO_3^-$ group is connected to its two adjacent neighbours by strong hydrogen bonds (O5—H5···O4) to build a two-dimensional network along the c direction. Some similarities may be observed between the present atomic arrangement and the corresponding dihydrogenphosphites investigated earlier (Bendheif *et al.*, 2003; William & Harrison, 2003). The guanine base occurs as the guaninium cation, $[C_5H_6N_5O]^+$, and we observe that only the imino group of the imidazolyl portion (N7) has been protonated in the reaction with the phosphorous acid, while the imino group of the pyrimidine moity (N3) is not protonated, as was observed in guaninium dinitrate dihydrate (Bouchouit *et al.*, 2002) and guaninium sulfate monohydrate (Cherouana *et al.*, 2003). The guaninium organic cations are connected to $H_2PO_3^-$ anions in two ways (in the following discussion symmetry codes are as in Table 2): (i) *via* a strong hydrogen bond nearly situated in their plane (N9—

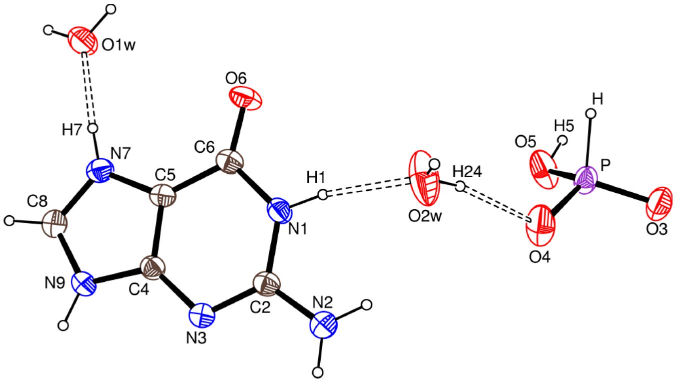


Figure 1
An *ORTEP*-3 (Farrugia, 1997) view, with the atomic labelling scheme, showing the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level.

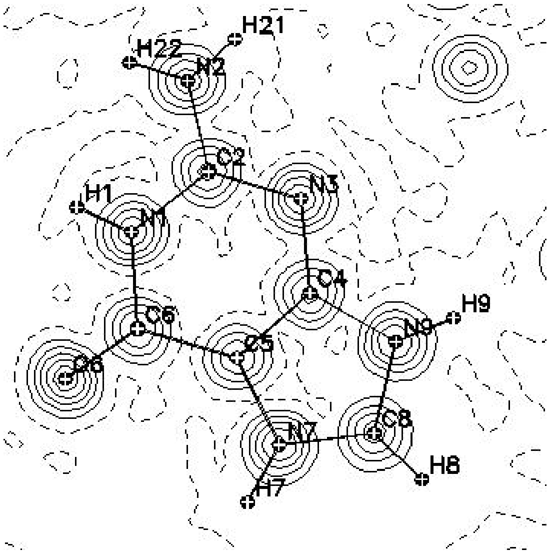


Figure 2
Observed deformation electron density in the cation plane.

N9···O3^{iv}) and (ii) *via* a long hydrogen bond (N2—H2*B*···O3^{iii}). When cations possess hydrogen-donor and hydrogen-acceptor functional groups, long hydrogen bonds occur between them; they are joined through only one hydrogen bond from the amino group N2 towards the imino group N3 (N2—H2*A*···N3^{ii}), so as to form infinite layers spreading along the [101] direction. A deformation electron-density map calculated from the observed X-ray structure factors (Fig. 2) showed significantly that the imidazolyl and pyrimidine rings are closely coplanar, their deviation from planarity being evidenced by the torsion angles. Water molecules play an important role in the cohesion and the stability of the crystal structure. The first water molecule (O1*W*) is involved in three hydrogen bonds connecting two guaninium cations *via* O1*W*···H7—N7 and O1*W*—H11···O6^{v}, and one phosphite anion *via* O1*W*—H12···O4^{vi}, while the second water molecule (O2*W*) is bonded to two phosphite anions *via* O2*W*—H24···O4 and O2W—H23···O3^{vii} and to the guaninium base *via* O2*W*···H1—N1 and O2*W*···H2*B*—N2. No hydrogen bonds between water molecules were observed.

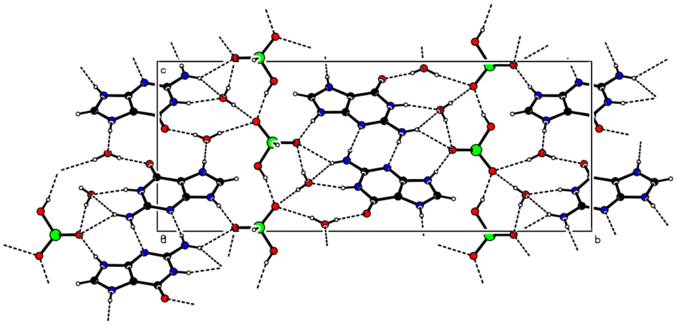


Figure 3
PLATON (Spek, 2003) view of the title compound, showing the intricate hydrogen-bond network, as dashed lines, between anions, cations and water molecules.

Experimental

The title compound was prepared by slow evaporation, at room temperature, of a dilute aqueous solution containing the base guanine and phosphorous acid in a stoichiometric ratio of 1:1. A few days later, crystals had grown as white needles.

Crystal data

$C_5H_6N_5O^+ \cdot H_2O_3P^- \cdot 2H_2O$
$M_r = 269.17$
Monoclinic, $P2_1/c$
$a = 4.7340$ (2) Å
$b = 24.0450$ (3) Å
$c = 9.5050$ (4) Å
$\beta = 98.860$ (4)°
$V = 1069.03$ (7) Å^3
$Z = 4$

$D_x = 1.672$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10263 reflections
$\theta = 2.3$–26.0°
$\mu = 0.29$ mm^{-1}
$T = 293$ (2) K
Needle, white
0.60 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ scans
Absorption correction: none
10263 measured reflections
1978 independent reflections
1722 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.047$
$\theta_{\rm max} = 26.0°$
$h = -5 \rightarrow 5$
$k = -29 \rightarrow 29$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.082$
$S = 1.06$
1978 reflections
170 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.3254P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.36$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O3—P	1.4905 (13)	O5—P	1.5580 (14)
O4—P	1.4989 (14)	P—H	1.332 (19)
O3—P—O4	117.40 (8)	O3—P—H	106.6 (9)
O3—P—O5	111.87 (8)	O4—P—H	110.8 (8)
O4—P—O5	107.33 (8)	O5—P—H	101.8 (8)
N3—C4—C5—N7	−179.49 (15)	C4—C5—C6—O6	−178.47 (17)
N9—C4—C5—N7	0.04 (18)	N7—C5—C6—N1	179.37 (16)
N3—C4—C5—C6	−0.4 (3)	O6—C6—N1—C2	179.65 (15)
N9—C4—C5—C6	179.14 (14)	N3—C4—N9—C8	179.81 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O4^{i}	0.82	1.74	2.5501 (19)	167
N1—H1···O2W	0.86	1.94	2.784 (2)	166
N2—H2A···N3^{ii}	0.86	2.12	2.976 (2)	173
N2—H2B···O2W	0.86	2.48	3.189 (2)	140
N2—H2B···O3^{iii}	0.86	2.59	3.131 (2)	122
N7—H7···O1W	0.86	1.81	2.6639 (19)	176
N9—H9···O3^{iv}	0.86	1.86	2.7165 (19)	172
O1W—H11···O6^{v}	0.832 (15)	1.917 (15)	2.7359 (18)	168 (2)
O1W—H12···O4^{vi}	0.813 (15)	2.175 (16)	2.929 (2)	154 (2)
O2W—H23···O3^{vii}	0.804 (17)	2.053 (17)	2.844 (2)	168 (3)
O2W—H24···O4	0.800 (17)	2.150 (17)	2.940 (2)	170 (3)

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

The H atoms were located in an electron-density difference map. The H atoms attached to C, O and N atoms were placed in calculated positions (C—H = 0.96 Å, O—H = 0.82 Å and N—H = 0.86 Å) and were refined using a riding model, with $U_{\rm iso}$ 1.2 times $U_{\rm eq}$ of the parent atoms. The H atoms of the water molecules were refined with O—H distances restrained to 0.84 (1) Å and H···H distances restrained to 1.37 (1) Å, with displacement parameters fixed at 1.2 times those of their parent atoms. These restraints ensure a reasonable geometry for the water molecules. The coordinates of the H atom attached to phosphorous were freely refined, with displacement parameters fixed at 1.2 times those of the P atom.

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

This work is supported by Mentouri-Constantine University, Algeria. We thank Dr M. Pierrot and Dr M. Giorgi from LBS–UMR 6517, Faculté des Sciences et Techniques de Saint Jérôme, Avenue Escadrille Normandie Niemen, 13397 Marseille Cedex 20, France, for diffraction facilities.

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