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[1-(Hydroxyethylammonio)propyl]phosphonate

Boris Shivachev,[a] Rosica Petrova,[a]* Krassimir Kossev[a] and Kolio Troev[b]

[a]Bulgarian Academy of Sciences, CL of Mineralogy and Crystallography, Acad. G. Bonchev Street, Building 107, 1113 Sofia, Bulgaria, and [b]Bulgarian Academy of Sciences, Institute of Polymers, Acad. G. Bonchev Street, Building 103A, 1113 Sofia, Bulgaria

Correspondence e-mail: rosipnikolova@abv.bg

Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.123
Data-to-parameter ratio = 16.2

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

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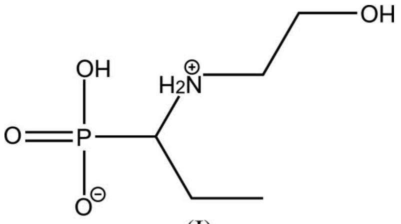
The molecule of the title compound, $C_5H_{14}NO_4P$, exists as a zwitterion rather than as [1-(hydroxyethylamino)propyl]-phosphonic acid, with the N atom of the amino group protonated and the phosphonic acid group negatively charged. In the crystal structure, the molecules are linked *via* extensive hydrogen bonding, forming layers parallel to (100).

Comment

The structural characteristics of α-aminophosphonic acids are interesting due to their potential biological activity (Neuzil *et al.*, 1980; Chen *et al.*, 1994). Recently, we began an investigation of new phosphomycin analogues and their biological activities. The synthesis of the title compound, (I), and its disodium salt has been reported previously (Troev *et al.*, 1999). This paper describes the crystal structure of (I).



(I)

The molecule of (I) exists as a zwitterion, the amino group being protonated and the phosphonic acid group being ionized (Fig. 1). The P—O2 and P—O3 bond distances show similar values, of 1.501 (2) and 1.505 (2) Å, respectively, indicating that the negative charge is nearly equally distributed between both O atoms. The molecule has an extended structure, as seen from the torsion angles of the P—C1—N1—C4—C5 backbone (Table 1). The α-ethyl and hydroxy groups are oriented on the same side of the backbone.

In the crystal structure, molecules of (I) face each other in an alternate end-to-end fashion, so that oppositely charged fragments are adjacent to each other. The molecules are linked *via* N—H···O and O—H···O hydrogen bonds (Table 2) to form ribbons running along the *b* axis (Fig. 2). Each pair of phosphonic acid groups from neighbouring chains is linked *via* an O1—H1···O3^{iii} hydrogen bond, to form layers parallel to (100). Thus, eight-membered rings of the type P—O1—H1*D*···O3^{iii}—P^{iii}—O1^{iii}—H1*D*^{iii}···O3 occur in the layers [symmetry code (iii) given in Table 1]. Similar rings are formed between phosphonate groups in other aminophosphonic acids (Weakley, 1976; Sawka-Dobrowolska *et al.*, 1993; Merz & Knüfer, 2002; Fernández & Vega, 2003).

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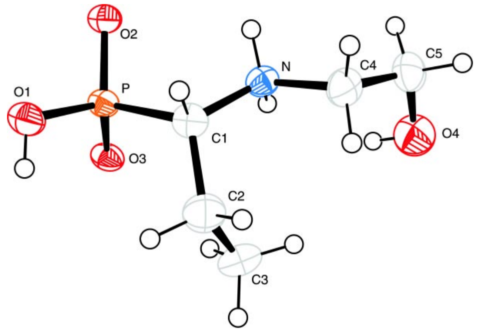

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Experimental

Compound (I) was synthesized by alkaline hydrolysis of 3-ethyl-2-hydroxy-2-oxo-1,4,2-oxaphosphorinane, as described by Troev *et al.* (1999). Crystals suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution.

Crystal data

$C_5H_{14}NO_4P$
$M_r = 183.14$
Monoclinic, $P2_1/c$
$a = 9.525$ (3) Å
$b = 5.992$ (3) Å
$c = 14.817$ (2) Å
$\beta = 94.77$ (2)°
$V = 842.7$ (5) Å^3
$Z = 4$
$D_x = 1.444$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
$\theta = 19.9$–$21.1°$
$\mu = 0.30$ mm^{-1}
$T = 290$ K
Prism, colourless
0.28 × 0.28 × 0.20 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Non–profiled $\omega/2\theta$ scans
Absorption correction: none
1757 measured reflections
1654 independent reflections
1305 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\rm max} = 26.0°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 7$
$l = -18 \rightarrow 18$
3 standard reflections
every 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.123$
$S = 0.88$
1654 reflections
102 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 1.1953P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.007 (2)

Table 1
Selected geometric parameters (Å, °).

C1—P	1.830 (3)	O2—P	1.5013 (19)
O1—P	1.5590 (19)	O3—P	1.5046 (19)
P—C1—N1—C4	178.3 (2)	C1—N1—C4—C5	161.2 (2)

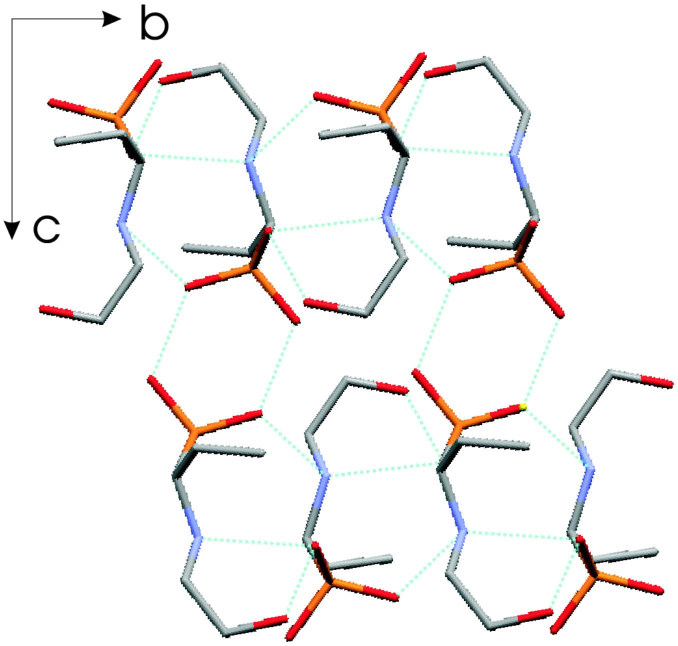

Figure 2
A projection of the crystal structure on the *bc* plane, showing the hydrogen-bonding network (dotted lines).

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4C···O2$^{\rm i}$	0.82	2.02	2.807 (3)	161
N1—H1B···O2$^{\rm i}$	0.90	1.86	2.742 (3)	165
N1—H1C···O3$^{\rm ii}$	0.90	2.02	2.873 (3)	157
O1—H1D···O3$^{\rm iii}$	0.82	1.85	2.555 (3)	143

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

The hydroxyl H atoms were placed in calculated positions and refined as riding, with O—H distances of 0.82 Å. H atoms bonded to N and C atoms were positioned geometrically and refined as riding, with N—H distances of 0.90 Å and C—H distances of 0.96–0.98 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom).

Data collection: *CAD-4 EXPRESS* (Enraf-Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WINGX* (Farrugia, 1999).

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