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## Crystal Structure

Communications
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## [(5-Bromopyridinium-2-ylamino)(phosphono)methyl]phosphonate

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The title compound, $\mathrm{C}_{6} \mathrm{H}_{9} \mathrm{BrN}_{2} \mathrm{O}_{6} \mathrm{P}_{2}$, a micromolar inhibitor of the farnesyl pyrophosphate synthase, is a $Z$-isomer zwitterion with one negative phosphonate group and a protonated pyridine N atom. Two types of ribbons, both parallel to the $a$ axis, formed by several centrosymmetrically related $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ and $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds are generated in the crystal structure. The resulting two-dimensional (001) 'double-layered' networks are joined into a threedimensional network via inversion-related halogen-oxygen interactions.

## Comment

Nitrogen-containing bisphosphonates are the subject of considerable interest because they have a wide range of potential applications, ranging from agriculture to medicine. It was only recently found that their mode of action in humans, parasites and plants relies on inhibition of the same enzyme of the mevalonate/isoprenoid pathway, namely the farnesyl pyrophosphate synthase (FPPS) (van Beek et al., 1999; Martin et al., 1999; Cheng \& Oldfield, 2004; Sanders et al., 2005; Ling et al., 2005; Cromartie et al., 1999).


The title compound, (I), is a member of the $N$-(2-pyridyl)-aminomethane-1,1-diphosphonic acid family. These compounds, first developed by Nissan as herbicides (Suzuki et al., 1979), have recently been shown to rank among highly active inhibitors of FPPS (Ghosh et al., 2004; Sanders et al., 2003). Spectroscopic and X-ray studies have revealed an interesting relationship between the topology of a substituent on the pyridyl ring and conformational preferences of this subclass of acids (Matczak-Jon et al., 2001, 2006; Matczak-Jon, 2005; Szabo et al., 2002; Sanders et al., 2003). The placement of the
substituent at the 4 - or 5 -position of the ring results in the predominance of the $Z$ over the $E$ geometrical isomer in solution and, as a result, the predominant form crystallizes in the solid state. By contrast, the 3-pyridyl-substituted compounds prefer the opposite $E$ geometry in both solution and the solid state (Matczak-Jon et al., 2001; Szabo et al., 2002).

We report here the results of our single-crystal X-ray study of (I), and compare the results with those previously obtained for the $N$-(5-methyl-2-pyridyl)- [Cambridge Structural Database (CSD; Allen, 2002) refcode QURYEH (Matczak-Jon et al., 2001)] and $N$-(5-chloro-2-pyridyl)- (Sanders et al., 2003; CSD refcode BEKCAW) derivatives, which unlike (I) contain two instead of one crystallographically independent zwitterion in the asymmetric unit.

Compound (I) is a zwitterion with one of the phosphonic acid groups deprotonated and pyridyl atom N 2 protonated (Fig. 1); this situation is common for this subclass of acids (Matczak-Jon et al., 2001, 2006; Sanders et al., 2003; Szabo et al., 2002). Atoms N1 and C1 are both coplanar with the pyridyl ring because of the formal $s p^{2}$ hybridization of atom N1. This results in a partial double-bond character of the $\mathrm{C} 2-\mathrm{N} 1$ linkage, which is reflected in the difference between its length and the length of the $\mathrm{C} 1-\mathrm{N} 1$ bond, which is typical for a single $\mathrm{C}-\mathrm{N}$ bond (Table 1). The $\mathrm{C} 1-\mathrm{N} 1-\mathrm{C} 2-\mathrm{N} 2$ torsion angle indicates that atom C 1 is only slightly displaced from the pyridyl ring plane [the distance of atom C 1 from that plane is 0.09 (2) $\AA$ ]. As expected, (I) adopts the same $Z$ geometry as the related 5-methyl and 5-chloro derivatives. This is reflected in the $\mathrm{C} 1-\mathrm{N} 1-\mathrm{C} 2-\mathrm{C} 3$ torsion angle (see Table 1 ), which can be compared with values of 3.7 (12) and 5.9 (12) ${ }^{\circ}$, and 6.5 (11) and $13.4(11)^{\circ}$, respectively, in the two crystallographically independent molecules of the 5-methyl- and 5-chloro-substituted compounds.

The geometry of the diphosphonate fragment is similar to that observed previously (Matczak-Jon et al., 2001, 2006). The $\mathrm{O} 1-\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2-\mathrm{O} 5$ sequence with one protonated and one deprotonated O atom reveals a typical almost planar W conformation. Accordingly, every P atom is oriented antiperiplanar ( ap ) to one of the O atoms from the adjacent phosphonic/phosphonate group and synclinal to the remaining O atoms from that group. The orientation of the diphosphonate group in relation to the rest of the molecule is additionally stabilized by an intramolecular $\mathrm{N} 1-\mathrm{H} 2 \cdots \mathrm{O} 3$ hydrogen bond. The formation of such an intramolecular

## Figure 1



The molecular structure of (I) showing the atom-numbering scheme and the intramolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bond. Displacement ellipsoids are drawn at the $50 \%$ probability level.
hydrogen bond, observed also in the $Z$-isomeric 4-methyl derivative (Matczak-Jon et al., 2006) and the E-isomeric 3methyl (Szabo et al., 2002) and 3-carboxy derivatives (Matczak-Jon et al., 2001), is a common feature of most of the aminomethane-1,1-diphosphonic acids studied to date (Matczak-Jon et al., 2005). As shown by the values of the C2$\mathrm{N} 1-\mathrm{C} 1-\mathrm{P} 1$ and $\mathrm{C} 2-\mathrm{N} 1-\mathrm{C} 1-\mathrm{P} 2$ torsion angles, both P atoms have an $a c$ orientation with respect to the pyridyl C 2 atom.

The geometry of both the phosphonic acid $\left(\mathrm{PO}_{3} \mathrm{H}_{2}\right)$ and the phosphonate $\left(\mathrm{PO}_{3} \mathrm{H}^{-}\right)$groups deviates significantly from an ideal tetrahedron (Table 1). This deviation is reflected in the values of the phosphonate $\mathrm{O} 1-\mathrm{P} 1-\mathrm{O} 2$ angles, in which the unprotonated O atoms are involved, and in the phosphonic acid $\mathrm{O} 4-\mathrm{P} 2-\mathrm{O} 6$ angles, involving the formal double $\mathrm{P}=\mathrm{O}$ bond. This configuration is consistent with what was previously observed for other members of this class of compounds (Matczak-Jon et al., 2001; Szabo et al., 2002; Sanders et al., 2003; Matczak-Jon \& Videnova-Adrabińska, 2005; Matczak-Jon et al., 2006).

The crystal packing in (I) is determined mainly by hydrogen bonds involving the phosphonic acid and phosphonate groups, which is a common feature of all the related compounds. The

(a)


(b)

Figure 2
The arrangement of the zwitterions in (I) within two types of ribbons (both along the $a$ axis) formed by adjacent chains interacting with each other via (a) centrosymmetric $\mathrm{O} 3-\mathrm{H} 3 \cdots \mathrm{O} 1^{\mathrm{i}}, \mathrm{N} 1-\mathrm{H} 2 \cdots \mathrm{O} 4^{\mathrm{iv}}$ and $\mathrm{N} 2-$ $\mathrm{H} 4 \cdots \mathrm{O} 4^{\mathrm{iv}}$ or $(b) \mathrm{O} 6-\mathrm{H} 6 \cdots \mathrm{O} 2^{\text {iii }}$ hydrogen bonds. The stabilizing $\mathrm{N} 1-$ $\mathrm{H} 2 \cdots \mathrm{O} 3$ interactions are also shown. Symmetry codes are given in Table 2.

W conformation of the $\mathrm{O} 1-\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2-\mathrm{O} 5$ sequence enables atoms O 5 and O 1 from adjacent molecules to participate in strong $\mathrm{O} 5-\mathrm{H} 5 \cdots \mathrm{O} 1^{\mathrm{ii}}$ hydrogen bonds (the geometry and symmetry codes are listed in Table 2). Such direct $a$-axis translation generates infinite chains of zwitterions (Fig. 2a), which is a common structural phenomenon for $N$-(5-methyl-2-pyridyl)-, (Matczak-Jon et al., 2001), $N$-(5-chloro-2-pyridyl)- (Sanders et al., 2003), $N$-(4-methyl-2-pyridyl)and non-substituted $N$-(2-pyridyl)aminomethane-1,1-diphosphonic acid (Matczak-Jon et al., 2006), but not for the 3-methyl and 3-carboxyl derivatives and the sodium salt of the 5-chlorosubstituted compound (Sanders et al., 2003).

The head-to-head arrangement of the molecules in adjacent chains enables the diphosphonate and diphosphonic acid groups to interact with each other to form ribbons (Fig. 2). Two different types of ribbons, both parallel to the $a$ axis, can be distinguished in the crystal structure of (I). Each zwitterion from one chain interacts with two others from an adjacent chain via several different hydrogen bonds. The centrosymmetric $\mathrm{O} 3-\mathrm{H} 3 \cdots \mathrm{O} 1^{i}$ contact with one zwitterion generates an $R_{2}^{2}(8)$ ring motif. Additional $R_{2}^{2}(10)$ and $R_{2}^{1}(6)$ rings are formed along the ribbon by bifurcated centrosymmetric $\mathrm{N} 1-\mathrm{H} 2 \cdots \mathrm{O} 4^{\text {iv }}$ and $\mathrm{N} 2-\mathrm{H} 4 \cdots \mathrm{O} 4^{\text {iv }}$ contacts to the same O 4 atom of another zwitterion. Such ribbons (Fig. 2a) are also observed in $N$-(4-methyl-2-pyridyl)aminomethane-1,1-diphosphonic acid (Matczak-Jon et al., 2006). On the other hand, pairs of zwitterions from adjacent chains are linked to each other by strong phosphonic-phosphonate $\mathrm{O} 6-\mathrm{H} 6 \cdots \mathrm{O} 2^{\text {iii }}$ hydrogen bonds. These, in combination with the O5$\mathrm{H} 5 \cdots \mathrm{O} 1^{\text {ii }}$ chain-forming interactions, give rise to $R_{2}^{2}(12)$ and $R_{4}^{4}(16)$ rings and another type of ribbon, shown in Fig. 2(b). The arrangement of the molecules within these ribbons is almost identical to that observed in $N$-(2-pyridyl)amino-methane-1,1-diphosphonic acid (Matczak-Jon et al., 2006).

As a result, a two-dimensional (001) 'double-layered' network is formed, which in turn interacts with the others via short halogen-oxygen interactions about inversion centres,


Figure 3
Adjacent chains from two different ribbons joined by $\mathrm{Br} \cdots \mathrm{O}^{\text {vii }}$ interactions (dashed lines) $\left[\mathrm{Br} \cdots \mathrm{O}^{\text {vii }}=2.967\right.$ (2) $\AA, \mathrm{C} 5-\mathrm{Br} \cdots \mathrm{O} 1^{\text {vii }}=$ $165.6(1)^{\circ}$ and $\mathrm{Br} \cdots \mathrm{O} 1^{\mathrm{vii}}-\mathrm{P} 1^{\mathrm{vii}}=126.8(1)^{\circ}$; symmetry code: (vii) $-x+2$, $-y+2,-z+2]$.

## organic compounds

with $\mathrm{Br} \cdots \mathrm{O}$ distances of 2.967 (2) $\AA$ and angular parameters consistent with the values usually observed for the halogen bonds (see Fig. 3). This gives rise to a three-dimensional network of zwitterions in the crystal structure of (I). It is worth noting that similar, but much weaker, halogen-oxygen interactions were also observed in the 5-chloro analogue, in which one of the two crystallographically independent zwitterions exhibited a $\mathrm{Cl} \cdots \mathrm{O}$ distance of about $3.17 \AA$ (Sanders et al., 2003).

## Experimental

Compound (I) was synthesized according to previously described procedures (Sołoducho et al., 1997). Crystals of (I) were obtained by slow evaporation of an aqueous solution at room temperature. NMR ( $\mathrm{D}_{2} \mathrm{O}, \mathrm{pH}=4.8$ ); ${ }^{1} \mathrm{H}$ NMR (p.p.m.): $\delta \mathrm{H}(1) 4.08\left({ }^{3} \mathrm{~J}_{\mathrm{PH}}=19.2 \mathrm{~Hz}\right.$ ), $\delta \mathrm{H}(31) 6.88, \delta \mathrm{H}(41) 7.48, \delta \mathrm{H}(61) 7.86 ;{ }^{13} \mathrm{C}$ NMR (p.p.m.): $\delta \mathrm{C} 151.39$ $\left({ }^{3} J_{\mathrm{PC}}=129.0 \mathrm{~Hz}\right), \delta \mathrm{C} 2152.78\left({ }^{3} J_{\mathrm{PC}}=4.0 \mathrm{~Hz}\right), \delta \mathrm{C} 3105.46, \delta \mathrm{C} 4137.72$, $\delta \mathrm{C} 5$ 114.11, $\delta \mathrm{C} 6144.91 ;{ }^{31} \mathrm{P}$ NMR (p.p.m.): $\delta \mathrm{P} 12.89$.

## Crystal data

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C6}\mp@subsup{\textrm{H}}{9}{}\mp@subsup{\textrm{BrN}}{2}{}\mp@subsup{\textrm{O}}{6}{}\mp@subsup{\textrm{P}}{2}{
Mr=347.00
Triclinic, P\overline{1}
a=7.224 (2) A
b=8.701 (2) \AA
c=10.382 (3) A
\alpha=103.51 (3) }\mp@subsup{}{}{\circ
\beta=98.97 (3)
\gamma=110.98(3)
V=571.5 (3) \AA}\mp@subsup{\AA}{}{3
```


## $Z=2$

$D_{x}=2.017 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation
Cell parameters from 8247
reflections
$\theta=4.9-38.7^{\circ}$
$\mu=3.90 \mathrm{~mm}^{-1}$
$T=100$ (2) K
Plate, colourless
$0.16 \times 0.06 \times 0.02 \mathrm{~mm}$

## Data collection

Oxford Xcalibur PX $\kappa$-geometry
diffractometer with an Onyx
CCD detector
$\omega$ and $\varphi$ scans
Absorption correction: analytical
(CrysAlis $R E D ;$ Oxford
Difffraction, 2003)
$T_{\min }=0.643, T_{\max }=0.940$

9823 measured reflections 3016 independent reflections
2575 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.037$
$\theta_{\text {max }}=29.0^{\circ}$
$h=-7 \rightarrow 9$
$k=-11 \rightarrow 11$
$l=-14 \rightarrow 14$

Table 1
Selected geometric parameters $\left(\AA^{\circ},{ }^{\circ}\right)$.

| P1-O1 | 1.517 (2) | P2-O6 | 1.541 (2) |
| :---: | :---: | :---: | :---: |
| $\mathrm{P} 1-\mathrm{O} 2$ | 1.492 (2) | P2-C1 | 1.832 (3) |
| P1-O3 | 1.572 (2) | N1-C1 | 1.454 (3) |
| P1-C1 | 1.847 (3) | N1-C2 | 1.338 (3) |
| P2-O4 | 1.488 (2) | N2-C2 | 1.355 (3) |
| P2-O5 | 1.561 (2) | N2-C6 | 1.353 (3) |
| $\mathrm{O} 1-\mathrm{P} 1-\mathrm{O} 2$ | 116.76 (11) | O5-P2-O6 | 106.33 (10) |
| $\mathrm{O} 1-\mathrm{P} 1-\mathrm{O} 3$ | 110.28 (10) | $\mathrm{O} 4-\mathrm{P} 2-\mathrm{C} 1$ | 109.63 (11) |
| $\mathrm{O} 2-\mathrm{P} 1-\mathrm{O} 3$ | 111.44 (11) | $\mathrm{O} 5-\mathrm{P} 2-\mathrm{C} 1$ | 103.39 (11) |
| $\mathrm{O} 1-\mathrm{P} 1-\mathrm{C} 1$ | 107.20 (11) | O6-P2-C1 | 107.84 (11) |
| $\mathrm{O} 2-\mathrm{P} 1-\mathrm{C} 1$ | 108.16 (11) | $\mathrm{C} 1-\mathrm{N} 1-\mathrm{C} 2$ | 127.7 (2) |
| $\mathrm{O} 3-\mathrm{P} 1-\mathrm{C} 1$ | 101.82 (11) | $\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2$ | 114.1 (2) |
| $\mathrm{O} 4-\mathrm{P} 2-\mathrm{O} 5$ | 113.59 (10) | $\mathrm{P} 1-\mathrm{C} 1-\mathrm{N} 1$ | 107.9 (2) |
| O4-P2-O6 | 115.26 (11) | $\mathrm{P} 2-\mathrm{C} 1-\mathrm{N} 1$ | 108.5 (2) |
| $\mathrm{O} 1-\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2$ | -172.8 (2) | $\mathrm{O} 3-\mathrm{P} 1-\mathrm{C} 1-\mathrm{N} 1$ | -49.2 (2) |
| $\mathrm{O} 2-\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2$ | -46.1 (2) | $\mathrm{O} 4-\mathrm{P} 2-\mathrm{C} 1-\mathrm{N} 1$ | 57.2 (2) |
| $\mathrm{O} 3-\mathrm{P} 1-\mathrm{C} 1-\mathrm{P} 2$ | 71.4 (2) | $\mathrm{O} 5-\mathrm{P} 2-\mathrm{C} 1-\mathrm{N} 1$ | -64.2 (2) |
| $\mathrm{O} 4-\mathrm{P} 2-\mathrm{C} 1-\mathrm{P} 1$ | -63.1 (2) | $\mathrm{O} 6-\mathrm{P} 2-\mathrm{C} 1-\mathrm{N} 1$ | -176.6 (2) |
| $\mathrm{O} 5-\mathrm{P} 2-\mathrm{C} 1-\mathrm{P} 1$ | 175.5 (2) | $\mathrm{C} 2-\mathrm{N} 1-\mathrm{C} 1-\mathrm{P} 1$ | -141.2 (2) |
| $\mathrm{O} 6-\mathrm{P} 2-\mathrm{C} 1-\mathrm{P} 1$ | 63.1 (2) | $\mathrm{C} 2-\mathrm{N} 1-\mathrm{C} 1-\mathrm{P} 2$ | 94.7 (3) |
| $\mathrm{O} 1-\mathrm{P} 1-\mathrm{C} 1-\mathrm{N} 1$ | 66.6 (2) | $\mathrm{C} 1-\mathrm{N} 1-\mathrm{C} 2-\mathrm{N} 2$ | 179.5 (2) |
| $\mathrm{O} 2-\mathrm{P} 1-\mathrm{C} 1-\mathrm{N} 1$ | -166.7 (2) | $\mathrm{C} 1-\mathrm{N} 1-\mathrm{C} 2-\mathrm{C} 3$ | 0.5 (4) |

## Refinement

Refinement on $F^{2}$
H -atom parameters constrained
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.034$
$w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}^{2}\right)+(0.0331 P)^{2}\right]$
where $P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3$
$\omega R\left(F^{2}\right)=0.071$
$\Delta / \sigma)_{\text {max }}=0.001$
$S=1.08$
$\Delta \rho_{\text {max }}=0.91 \mathrm{e}^{\AA^{-3}}$
3016 reflections
$\Delta \rho_{\min }=-0.45 \mathrm{e}^{-3}$

Table 2
Hydrogen-bond geometry ( $\AA{ }^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{O} 3-\mathrm{H} 3 \cdots \mathrm{O} 1^{\mathrm{i}}$ | 0.84 | 1.80 | 2.607 (3) | 161 |
| $\mathrm{O} 5-\mathrm{H} 5 \cdots \mathrm{O} 1^{\text {ii }}$ | 0.84 | 1.72 | 2.559 (2) | 176 |
| O6-H6 $\cdots \mathrm{O}^{\text {iii }}$ | 0.84 | 1.70 | 2.538 (3) | 179 |
| $\mathrm{N} 1-\mathrm{H} 2 \cdots \mathrm{O} 3$ | 0.88 | 2.44 | 2.888 (3) | 112 |
| $\mathrm{N} 1-\mathrm{H} 2 \cdots \mathrm{O} 4^{\text {iv }}$ | 0.88 | 1.98 | 2.769 (3) | 149 |
| $\mathrm{N} 2-\mathrm{H} 4 \cdots \mathrm{O} 4^{\text {iv }}$ | 0.88 | 1.84 | 2.648 (3) | 152 |
| $\mathrm{C} 4-\mathrm{H} 41 \cdots \mathrm{O}^{\text {v }}$ | 0.95 | 2.47 | 3.382 (3) | 160 |
| $\mathrm{C} 4-\mathrm{H} 41 \cdots \mathrm{O}^{\text {v}}$ | 0.95 | 2.60 | 3.303 (3) | 131 |
| C6-H61 $\cdots \mathrm{O}^{\text {vi }}$ | 0.95 | 2.60 | 3.298 (3) | 131 |

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

All H atoms were found in difference Fourier maps. In the final refinement cycles, the H atoms were treated as riding atoms, with $\mathrm{O}-$ H distances of $0.84 \AA, \mathrm{~N}-\mathrm{H}$ distances of $0.88 \AA$, and $\mathrm{C}-\mathrm{H}$ distances of 0.95 or $1.00 \AA$, and with $U_{\text {iso }}(\mathrm{H})$ values of $1.5 U_{\text {eq }}(\mathrm{O})$ and $1.2 U_{\text {eq }}(\mathrm{N}, \mathrm{C})$.

Data collection: CrysAlis CCD (Oxford Diffraction, 2003); cell refinement: CrysAlis RED (Oxford Diffraction, 2003); data reduction: CrysAlis RED; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG3003). Services for accessing these data are described at the back of the journal.

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