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Bis(2-amino-5-chloropyridinium) dihydrogendiphosphate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 25.4

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

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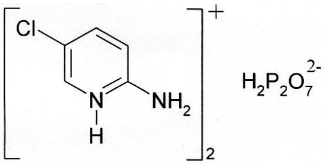
The title compound, $2C_5H_6ClN_2^+\cdot H_2P_2O_7^{2-}$, contains infinite $(H_2P_2O_7^{2-})_n$ ribbons extending along the *c* direction. The bridging O atom of the diphosphate anion is located on a twofold axis. The organic cations are anchored between planes parallel to *ac*, linking the ribbons into a three-dimensional network.

Comment

Recently, organic–inorganic hybrid materials have attracted more and more attention, especially when they are obtained by an appropriate choice of cation and anion, the ultimate hope being that such assemblies will lead to novel materials possessing interesting features and properties. An important strategy employed in studying such systems has been to take advantage of hydrogen-bond interactions between organic cations and inorganic anions, since they have been recognized as the most powerful force to generate supramolecular networks in one, two and three dimensions (Desiraju, 1989; Steiner, 2002). In this context, our aims have been focused on the salts of diphosphate groups and the organic salts of diphosphate groups. The title compound, (I), provides another example of this kind of compound.



(I)

The asymmetric unit of the title compound (Fig. 1) is composed of a 2-amino-5-chloropyridinium cation and one-half of a dihydrogendiphosphate anion. The bridging O atom of the diphosphate group is located on a twofold axis.

Our study shows the occurrence of hydrogen-bonding interactions between the anions and the cations associated with electrostatic and van der Waals weak interactions. In fact, the structure exhibits two kinds of hydrogen bonds (Table 1), *viz.* (i) O—H···O interactions leading to the formation of infinite $(H_2P_2O_7^{2-})_n$ ribbons extending along the *c* direction and (ii) N—H···O interactions originating from the NH^+ and NH_2 groups of the organic ions, interconnecting the inorganic ribbons.

A projection along the [110] direction (Fig. 2) clearly shows the organic cations sandwiched between the $(H_2P_2O_7^{2-})_n$ polymeric anions, whereas a projection along the *b* direction shows the layer composed of anions arranged in infinite ribbons parallel to the *c* direction (Fig. 3).

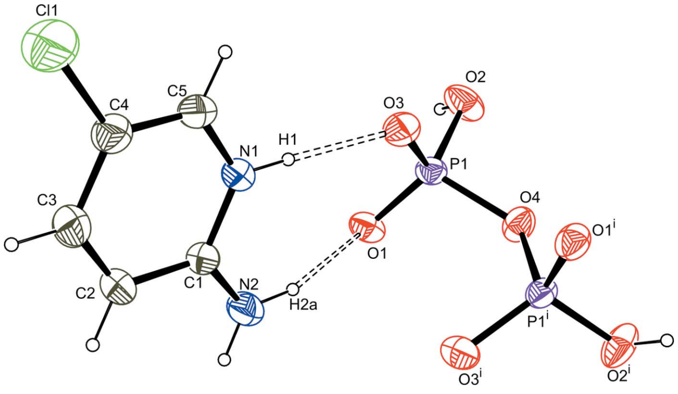


Figure 1
ORTEP-3 (Farrugia, 1997) view of the title compound, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. [Symmetry codes: (i) $-x, y, -z + \frac{1}{2}$].

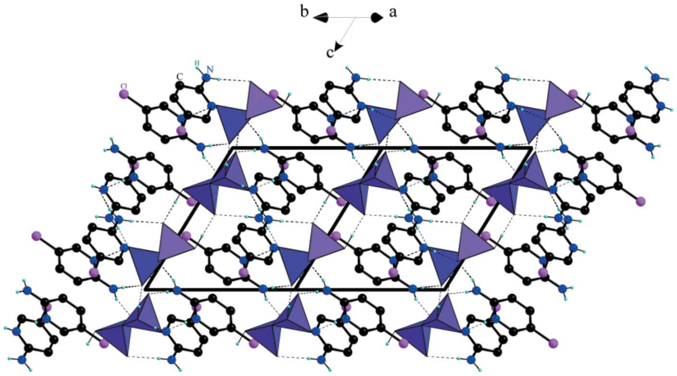


Figure 2
Projection of the structure along the [110] direction.

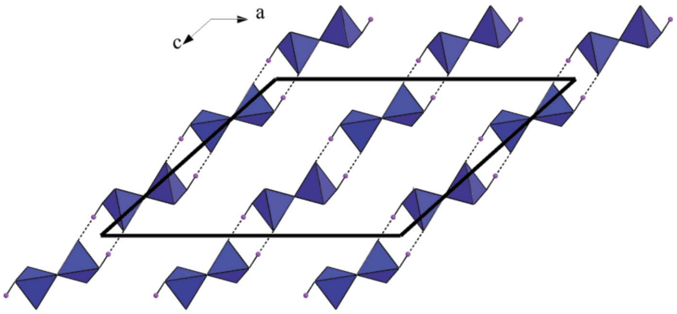


Figure 3
Projection of the $(H_2P_2O_7^{2-})_n$ polymeric anions running along the *c* axis.

The geometric parameters in the 2-amino-5-chloropyridinium cation are similar to those observed for other salts containing this organic cation (Ouslati *et al.*, 2005). As expected, the geometric parameters of the $H_2P_2O_7^{2-}$ anion agree with those previously observed for diphosphates with twofold symmetry (Charfi & Jouini, 1997; Averbuch-Pouchot & Durif, 1992).

Experimental

2-Amino-5-chloropyridine and $H_4P_2O_7$ in a 2:1 molar ratio in aqueous solution were mixed, with shaking, at low room temperature. The diphosphoric acid was produced from $Na_4P_2O_7$ by using an ion-exchange resin (Amberlite IR 120). The resulting solution was evaporated slowly at room temperature for several days until the formation of good quality prismatic single crystals.

Crystal data

$2C_5H_6ClN_2^+ \cdot H_2O_7P_2^{2-}$
$M_r = 435.10$
Monoclinic, $C2/c$
$a = 16.872\ (8)$ Å
$b = 11.144\ (3)$ Å
$c = 11.266\ (5)$ Å
$\beta = 128.55\ (3)°$
$V = 1656.6\ (14)$ Å^3
$Z = 4$
$D_x = 1.745$ Mg m^{-3}
Ag $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 9$–$11°$
$\mu = 0.33$ mm^{-1}
$T = 293$ K
Prism, colorless
$0.23 \times 0.17 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3057 measured reflections
2948 independent reflections
2589 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$
$h = -16 \rightarrow 25$
$k = 0 \rightarrow 16$
$l = -16 \rightarrow 16$
2 standard reflections every 400 reflections intensity decay: 0.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.112$
$S = 1.13$
2948 reflections
116 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 1.4425P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0150 (15)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2$\cdots$O1^i	0.82	1.77	2.574 (2)	165
N1—H1$\cdots$O3	0.86	1.83	2.6792 (18)	168
N2—H2$A\cdots$O1	0.86	2.04	2.8651 (19)	160
N2—H2$B\cdots$O3^{ii}	0.86	2.03	2.811 (2)	151

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

H atoms were treated as riding, with C—H = 0.93 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with U_{iso}(H) = $1.2U_{eq}$(C,N) and $1.5U_{eq}$(O).

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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