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2-Amino-5-methylpyridinium phosphate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.093
Data-to-parameter ratio = 13.1

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

The title compound, $C_6H_9N_2^+\cdot H_2PO_4^-$, consists of 2-amino-5-methylpyridinium cations and $H_2PO_4^-$ anions, which are held together by N—H···O hydrogen bonds.

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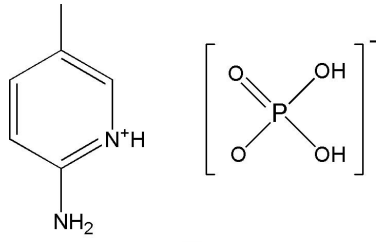
Comment

Previously, some 2-amino-*X*-methylpyridine (2A*X*MP, *X* indicating the methyl position) adducts have been synthesized in our laboratory, including 2A6MP–neoabietic acid (1/1) (Jin *et al.*, 2000), 2A3MP–phthalic acid (2/1) (Jin *et al.*, 2001), 2A3MP–maleic acid (2/3) (Jin *et al.*, 2002), 2A6MP–tetrachlorozincate(II) (Jin, Shun *et al.*, 2005) and 2-amino-5-methylpyridinium (2-amino-5-methylpyridine)trichlorozincate(II) (Jin, Tu *et al.*, 2005). Here a new compound, (I), has been synthesized from 2A5MP and phosphoric acid.



(I)

In the formula unit of the title compound, the 2-amino-5-methylpyridinium cation is linked to an $H_2PO_4^-$ anion by N1—H2*A*···O1 and N2—H2*N*···O2 hydrogen bonds (Fig. 1 and Table 2). N—H···O, O—H···O and C—H···O hydrogen bonds are instrumental in building the three-dimensional structure (Fig. 2 and Table 2).

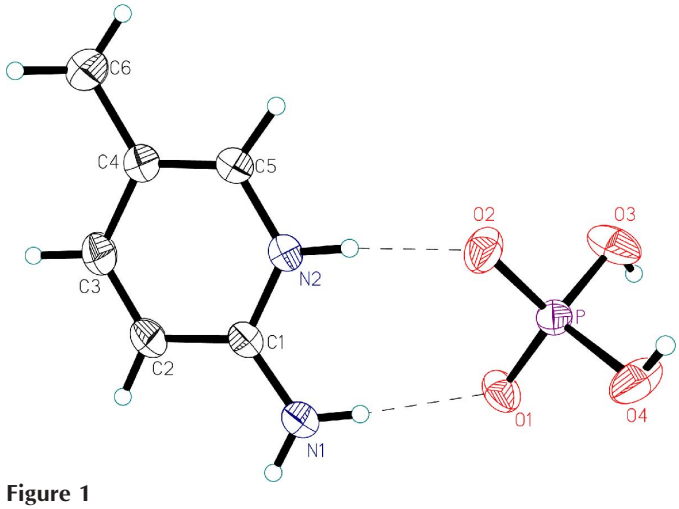


Figure 1
View of (I), with atom labels, showing 40% probability displacement ellipsoids. Hydrogen bonds are illustrated as dashed lines.

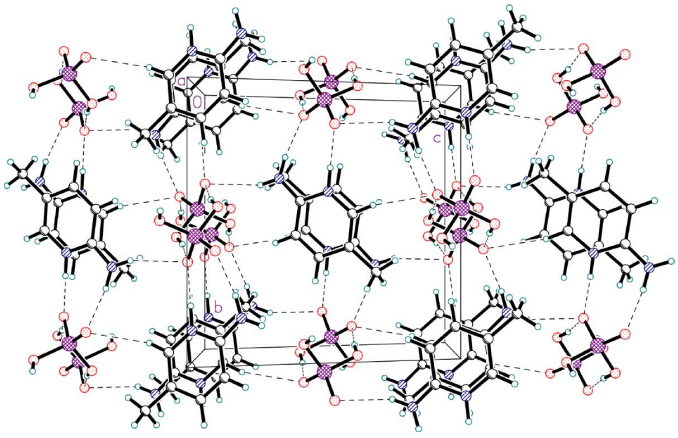


Figure 2
Packing diagram, viewed along the *a* axis. Hydrogen bonds are illustrated as dashed lines.

Experimental

Phosphoric acid and 2-amino-5-methylpyridine in a molar ratio of 1:1 were mixed and dissolved in sufficient ethanol by heating to a temperature at which a clear solution resulted. Crystals of (I) were formed by gradual evaporation of ethanol over a period of one week at 293 K.

Crystal data

$C_6H_9N_2^+\cdot H_2PO_4^-$
M_r = 206.14
Monoclinic, $P2_1/n$
a = 7.9850 (5) Å
b = 10.9104 (6) Å
c = 11.1556 (7) Å
β = 108.414 (2)°
V = 922.11 (10) Å^3
Z = 4
D_x = 1.485 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 71 reflections
θ = 2.7–27.5°
μ = 0.28 mm^{-1}
T = 293 (2) K
Block, colourless
0.45 × 0.45 × 0.31 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.880, T_{max} = 0.916
3577 measured reflections
2111 independent reflections
1664 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.093
S = 0.97
2111 reflections
162 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected interatomic distances (Å).

P—O1	1.5031 (11)	N2—C5	1.3677 (19)
P—O2	1.5071 (11)	C1—C2	1.402 (2)
P—O3	1.5566 (12)	C2—C3	1.358 (3)
P—O4	1.5555 (13)	C3—C4	1.420 (2)
N1—C1	1.322 (2)	C6—C4	1.502 (2)
N2—C1	1.3492 (18)	C4—C5	1.348 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2A···O1^{i}	0.84 (2)	1.97 (2)	2.789 (3)	164 (2)
N1—H1A···O2^{ii}	0.86 (2)	2.31 (2)	3.073 (2)	148 (2)
N2—H2N···O2^{i}	0.94 (2)	1.87 (2)	2.802 (2)	174 (2)
O3—H3O···O1^{iii}	0.90 (2)	1.65 (2)	2.550 (3)	174 (2)
O4—H4O···O2^{iv}	0.89 (2)	1.74 (2)	2.612 (3)	166 (2)
C5—H5···O1^{v}	1.00 (2)	2.59 (2)	3.464 (3)	146 (1)

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

All H atoms were located in a difference Fourier map and refined isotropically [C—H = 0.85 (3)–1.03 (3) Å].

Data collection: *PROCESS-AUTO* (Rigaku, 2001); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CrystalStructure*; molecular graphics: *SHELXTL* (Siemens, 1998); software used to prepare material for publication: *CrystalStructure*.

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