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2,4,6-Trimethylpyridinium dihydrogen phosphate

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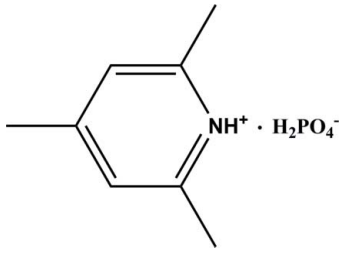
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.144; data-to-parameter ratio = 14.3.

In the title compound, $C_8H_9N^+\cdot H_2PO_4^-$, both the cation and anion have crystallographically imposed mirror symmetry (all atoms apart from one O atom lie on the mirror plane). In the crystal, anions and cations are linked by O—H···O and π–π stacking interactions [centroid–centroid distance = 3.4574 (6) Å], forming chains parallel to the b axis. Adjacent chains are further connected by N—H···O hydrogen bonds into a two-dimensional network.

Related literature

For background to the properties of pyridine salts as phase-transition dielectric materials, see: Fu *et al.* (2007, 2008, 2009); Fu & Xiong (2008).



Experimental

Crystal data

$C_8H_9N^+\cdot H_2O_4P^-$
M_r = 216.15
Monoclinic, $P2_1/m$
a = 8.6323 (17) Å
b = 6.7133 (13) Å
c = 8.6841 (17) Å
β = 100.99 (3)°
V = 494.02 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 298 K
0.30 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
5154 measured reflections
1229 independent reflections
1082 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.144
S = 1.18
1229 reflections
86 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3^{i}	0.85 (2)	1.76 (2)	2.6054 (19)	169 (2)
N1—H1A···O1	0.86	1.75	2.602 (3)	173

Symmetry code: (i) $-x, -y, -z+2$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2528).

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supplementary materials

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