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Ammonium benzenephosphonate

Zhen Lin,[a] Xiu-Qing Lei,[b] Sheng-Di Bai[b] and Seik Weng Ng[c]*

[a]Shanxi Vocational and Technical College of Biological Applications, Taiyuan 030031, Shanxi, People's Republic of China, [b]Institute of Applied Chemistry, Shanxi University, Taiyuan 030006, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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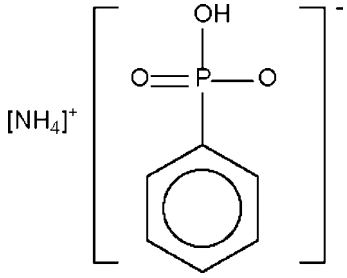
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.067; wR factor = 0.174; data-to-parameter ratio = 13.0.

In the crystal structure of the title salt, $NH_4^+.[(C_6H_5)P(O)_2(OH)]^-$ or $NH_4^+\cdot C_6H_6O_3P^-$, the N and O atoms interact *via* hydrogen bonds to generate a layer motif. The phenyl rings are stacked above and below this layer, sandwiching the hydrogen-bonded layer.

Related literature

For the crystal structure of benzenephosphonic acid, see: Weakley (1976); Mahmoudkhani & Langer (2002). For the crystal structure of the 1:1 co-crystal of ammonium benzenephosphonate and benzenephosphonic acid, see: Rao & Vidyasagar (2005).



Experimental

Crystal data

$NH_4^+\cdot C_6H_6O_3P^-$
M_r = 175.12
Orthorhombic, *Pbcn*
a = 31.122 (2) Å
b = 7.1249 (5) Å
c = 7.9441 (5) Å
V = 1761.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 (2) K
0.4 × 0.4 × 0.2 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.807, T_{max} = 0.947
7880 measured reflections
1565 independent reflections
1540 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.173
S = 1.27
1565 reflections
120 parameters
11 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.85 (1)	1.71 (2)	2.526 (3)	163 (4)
N1—H11···O2	0.85 (1)	1.91 (1)	2.762 (4)	175 (3)
N1—H12···O3^{ii}	0.85 (1)	1.99 (1)	2.814 (4)	164 (3)
N1—H13···O1^{iii}	0.85 (1)	2.09 (2)	2.940 (4)	173 (3)
N1—H14···O2^{iv}	0.85 (1)	1.93 (1)	2.775 (4)	177 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2441).

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supporting information

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S1. Comment

The title compound (Scheme I, Fig. 1) is a side-product in the synthesis of 2-methylphenylamidinium phenylphosphinate.

S2. Experimental

m-Tolunitrile (0.6 ml, 5 mmol) and lithium bis(trimethylsilyl)amide (0.83 g, 5 mmol) were dissolved in THF (30 ml) at 273 K. The yellow solution was cooled to 195 K. Dichlorophenylphosphine (0.7 ml, 5 mmol) was added. The solution was kept at this temperature for an hour before being allowed to react at room temperature overnight. The solvent was removed and the residue extracted with dichloromethane to give a light yellow oil. The oil was dissolved in acetonitrile (30 ml) and 30% hydrogen peroxide (0.56 cm l, 5 mmol) was added. After 24 h, the solution was filtered. Colorless crystals of 2-methylphenylamidinium phenylphosphinate were first obtained; the second crop yielded the title compound (yield 0.04 g).

S3. Refinement

The hydroxy and ammonium H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = N—H 0.85 (1) Å and H···H 1.39 (1) Å. Their temperature factors were freely refined. The aromatic H atoms were placed at calculated positions, and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

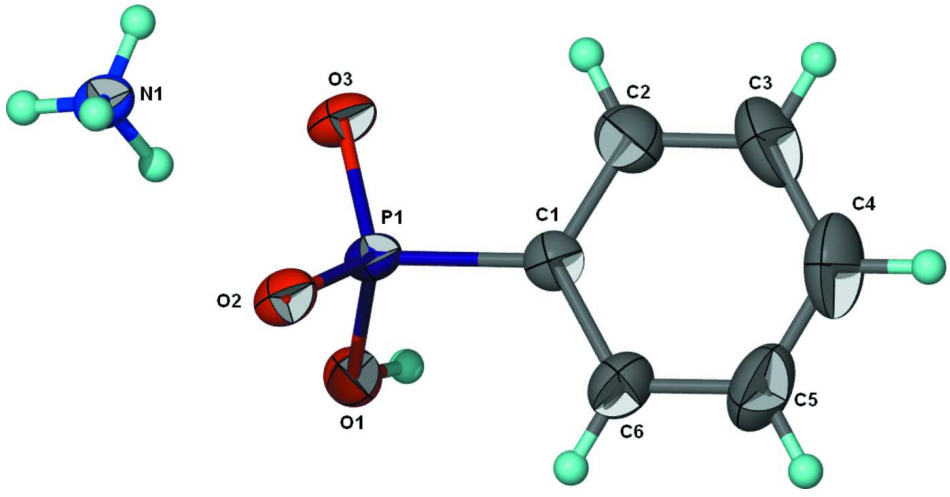

Figure 1

The molecular structure, showing the atom-numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

Ammonium benzenephosphonate

Crystal data

$NH_4^+ \cdot C_6H_6O_3P^-$
$M_r = 175.12$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 31.122$ (2) Å
$b = 7.1249$ (5) Å
$c = 7.9441$ (5) Å
$V = 1761.5$ (2) Å^3
$Z = 8$
$F(000) = 736$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3647 reflections
$\theta = 2.6$–$27.5°$
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Block, colorless
0.4 × 0.4 × 0.2 mm

Data collection

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.807$, $T_{max} = 0.947$
7880 measured reflections
1565 independent reflections
1540 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.3°$
$h = -37 \rightarrow 30$
$k = -8 \rightarrow 6$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.173$
$S = 1.27$
1565 reflections
120 parameters
11 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 2.2855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.42250 (3)	0.69330 (12)	0.59684 (10)	0.0317 (3)
O1	0.45014 (8)	0.6911 (4)	0.4300 (3)	0.0410 (7)
H1	0.4413 (14)	0.607 (4)	0.363 (4)	0.056 (13)*
O2	0.43772 (8)	0.8608 (3)	0.6936 (3)	0.0403 (6)
O3	0.42584 (8)	0.5088 (3)	0.6853 (3)	0.0431 (7)
N1	0.46015 (10)	0.8111 (4)	1.0270 (4)	0.0373 (7)
H11	0.4547 (9)	0.827 (4)	0.9228 (14)	0.053 (13)*
H12	0.4455 (8)	0.720 (3)	1.065 (3)	0.052 (13)*
H13	0.4869 (4)	0.786 (4)	1.038 (4)	0.043 (11)*
H14	0.4541 (9)	0.910 (2)	1.081 (3)	0.048 (12)*
C1	0.36793 (11)	0.7216 (5)	0.5282 (5)	0.0381 (8)
C2	0.33569 (14)	0.6096 (7)	0.5945 (6)	0.0566 (11)
H2	0.3423	0.5194	0.6751	0.068*

C3	0.29380 (15)	0.6318 (9)	0.5410 (8)	0.0742 (15)
H3	0.2722	0.5584	0.5879	0.089*
C4	0.28380 (16)	0.7611 (9)	0.4195 (8)	0.0802 (16)
H4	0.2556	0.7725	0.3822	0.096*
C5	0.31517 (17)	0.8734 (8)	0.3528 (7)	0.0755 (15)
H5	0.3082	0.9619	0.2711	0.091*
C6	0.35723 (14)	0.8548 (6)	0.4073 (6)	0.0565 (11)
H6	0.3785	0.9320	0.3627	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0411 (5)	0.0288 (5)	0.0252 (5)	−0.0007 (3)	−0.0013 (3)	0.0022 (3)
O1	0.0427 (14)	0.0516 (16)	0.0289 (13)	−0.0082 (12)	−0.0003 (11)	−0.0042 (11)
O2	0.0564 (15)	0.0319 (12)	0.0326 (13)	−0.0039 (11)	−0.0083 (11)	−0.0017 (10)
O3	0.0605 (16)	0.0326 (13)	0.0362 (13)	0.0034 (12)	−0.0034 (11)	0.0064 (11)
N1	0.0479 (19)	0.0322 (16)	0.0318 (16)	−0.0016 (13)	−0.0031 (14)	0.0005 (13)
C1	0.0419 (19)	0.0355 (18)	0.0369 (19)	0.0011 (15)	0.0009 (15)	−0.0046 (15)
C2	0.054 (2)	0.060 (3)	0.056 (3)	−0.008 (2)	0.001 (2)	0.002 (2)
C3	0.041 (2)	0.092 (4)	0.089 (4)	−0.011 (2)	0.004 (2)	−0.011 (3)
C4	0.045 (3)	0.099 (4)	0.097 (4)	0.016 (3)	−0.018 (3)	−0.019 (4)
C5	0.066 (3)	0.078 (3)	0.082 (3)	0.017 (3)	−0.026 (3)	0.011 (3)
C6	0.055 (3)	0.055 (2)	0.060 (3)	0.005 (2)	−0.011 (2)	0.014 (2)

Geometric parameters (Å, º)

P1—O3	1.494 (2)	C1—C6	1.391 (5)
P1—O2	1.497 (2)	C2—C3	1.380 (7)
P1—O1	1.580 (3)	C2—H2	0.9300
P1—C1	1.795 (4)	C3—C4	1.370 (8)
O1—H1	0.85 (1)	C3—H3	0.9300
N1—H11	0.85 (1)	C4—C5	1.369 (8)
N1—H12	0.85 (1)	C4—H4	0.9300
N1—H13	0.85 (1)	C5—C6	1.385 (6)
N1—H14	0.85 (1)	C5—H5	0.9300
C1—C2	1.386 (6)	C6—H6	0.9300
O3—P1—O2	115.98 (14)	C3—C2—C1	120.1 (5)
O3—P1—O1	110.38 (14)	C3—C2—H2	120.0
O2—P1—O1	105.45 (14)	C1—C2—H2	120.0
O3—P1—C1	107.91 (16)	C4—C3—C2	120.6 (5)
O2—P1—C1	111.44 (16)	C4—C3—H3	119.7
O1—P1—C1	105.14 (15)	C2—C3—H3	119.7
P1—O1—H1	111 (3)	C5—C4—C3	120.3 (5)
H11—N1—H12	109.6 (14)	C5—C4—H4	119.9
H11—N1—H13	108.8 (14)	C3—C4—H4	119.9
H12—N1—H13	109.2 (14)	C4—C5—C6	119.8 (5)
H11—N1—H14	109.7 (14)	C4—C5—H5	120.1

H12—N1—H14	110.1 (14)	C6—C5—H5	120.1
H13—N1—H14	109.5 (14)	C5—C6—C1	120.5 (4)
C2—C1—C6	118.8 (4)	C5—C6—H6	119.8
C2—C1—P1	120.3 (3)	C1—C6—H6	119.8
C6—C1—P1	120.9 (3)		
O3—P1—C1—C2	15.9 (4)	P1—C1—C2—C3	−179.9 (4)
O2—P1—C1—C2	−112.6 (3)	C1—C2—C3—C4	1.5 (8)
O1—P1—C1—C2	133.7 (3)	C2—C3—C4—C5	−1.7 (9)
O3—P1—C1—C6	−163.7 (3)	C3—C4—C5—C6	0.6 (9)
O2—P1—C1—C6	67.8 (4)	C4—C5—C6—C1	0.6 (8)
O1—P1—C1—C6	−45.9 (4)	C2—C1—C6—C5	−0.8 (7)
C6—C1—C2—C3	−0.3 (7)	P1—C1—C6—C5	178.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{i}	0.85 (1)	1.71 (2)	2.526 (3)	163 (4)
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Symmetry codes: (i) *x*, −*y*+1, *z*−1/2; (ii) *x*, −*y*+1, *z*+1/2; (iii) −*x*+1, *y*, −*z*+3/2; (iv) *x*, −*y*+2, *z*+1/2.