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3-Aminopropylphosphonic Acid

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Abstract. $C_3H_{10}NO_3P$, $M_r = 139{\cdot}01$, orthorhombic, $Pna2_1$, $a = 9{\cdot}495$ (2), $b = 7{\cdot}925$ (1), $c = 8{\cdot}017$ (1) Å, $Z = 4$, $D_m = 1{\cdot}53$ (by flotation), $D_x = 1{\cdot}53$ Mg m^{-3}; final $R = 0{\cdot}062$. The molecule exists as the zwitterion $H_3^+N-(CH_2)_3-PO_3H^-$. There are four independent hydrogen bonds in the structure; three are of the type N—H···O with lengths 2·811, 2·812 and 2·831 Å, and one is of the type O—H···O with length 2·522 Å.

Introduction. 3-Aminopropylphosphonic acid was prepared by a method developed by Dr R. Tyka at the Institute of Organic and Physical Chemistry, Technical University of Wrocław. Crystals suitable for X-ray analysis were colourless prisms. The space group and cell constants were obtained initially from Weissenberg photographs. The cell parameters were determined by least-squares refinement from the setting angles of 15 reflexions given by the automatic centring program [λ(Cu $K\alpha$) = 1·5418 Å]. All measurements for a crystal 0·08 × 0·15 × 0·15 mm were made on a Syntex $P2_1$ computer-controlled four-circle diffractometer equipped with a scintillation counter and graphite monochromator. 475 independent reflexions were measured up to $2\theta = 114{\cdot}0°$ with the variable θ–2θ scan technique. The scan rate varied from 3·0 to 20·0° min^{-1}, depending on the intensity. After each group of 15 reflexions the intensity of a standard was measured; no significant change was observed. The intensities were corrected for Lorentz and polarization factors, but not for absorption [μ(Cu $K\alpha$) = 3·44 mm^{-1}].

The structure was solved by the heavy-atom technique and refined anisotropically by full-matrix least squares. A difference synthesis revealed the positions of nine H atoms. The H atom of the OH group was not located. The coordinates of the H atoms and their isotropic thermal factor ($B = 3{\cdot}8$ Å^2) were not refined. The final $R = 0{\cdot}062$ and $R_w = 0{\cdot}081$ for 436 observed reflexions for which $F > 3{\cdot}92\sigma(F)$. For all 475 reflexions R and R_w are 0·066 and 0·081. The function minimized was $\sum w(|F_o| - |F_c|)^2$ with $w = 1/\sigma^2(F)$. Scattering factors for neutral atoms were taken from *International Tables for X-ray Crystallography* (1974). All calculations were performed with the Syntex *XTL* structure determination system on a Nova 1200

Table 1. *Positional parameters* (×10^4; *for* H ×10^3) *with e.s.d.'s in parentheses*

The atomic parameters of H were not refined; $B_{iso} = 3{\cdot}8$ Å^2.

	x	y	z
P	1559 (3)	2270 (1)	3500 (1)
O(1)	2769 (8)	3176 (11)	4570 (12)
O(2)	1809 (8)	2422 (11)	1653 (12)
O(3)	187 (8)	3063 (11)	4134 (13)
N	667 (10)	−3548 (12)	5087 (15)
C(1)	1665 (13)	65 (14)	4066 (18)
C(2)	465 (14)	−949 (13)	3220 (18)
C(3)	697 (15)	−2884 (14)	3303 (21)
H(1)	157	−7	530
H(2)	259	−42	370
H(3)	42	−59	200
H(4)	−44	−67	377
H(5)	166	−316	279
H(6)	−4	−347	262
H(7)	72	−483	498
H(8)	−23	−322	578
H(9)	149	−312	575

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computer with additional external disc memory. The final parameters are listed in Table 1.*

Discussion. The molecular structure and atom numbering are shown in Fig. 1, a projection down **a**. Bond distances and angles are given in Table 2.

No significant deviations from normal values of lengths and angles occur.

The C–H lengths vary from 0·99 to 1·02 Å and the N–H lengths from 1·0 to 1·02 Å. The angles involving the H atoms in the amino group range from 107·4 to 109·9°, and in the CH_2 groups from 107·8 to 110·5°.

The coordination around the P atom departs significantly from regular tetrahedral, the angles varying from 104·3 [O(3)–P–O(1)] to 115·3° [O(3)–P–O(2)]; these agree well with the values found in aminomethylphosphonic acid (β-AMPh) (Darriet, Darriet, Cassaigne & Neuzil, 1975) and in 2-aminoethylphosphonic acid (Okaya, 1966).

The P–O distances in the present compound appear to split into two groups: two short P–O bonds and one long P–OH bond. The P–O lengths of 1·505 (10) and 1·534 (9) Å agree within the limits of error with similar bonds in 2-aminoethylphosphoric acid (Kraut, 1961), β-ciliatine (Okaya, 1966), β-AMPh (Darriet *et al.*, 1975) and (aminomethyl)methylphosphinic acid (AMMPh) (Głowiak & Sawka-Dobrowolska, 1977). The P–OH length of 1·603 (9) Å is slightly longer (by 3σ) than the P–OH length in β-ciliatine (1·569 Å), 2-aminoethylphosphoric acid (1·557 Å), and β-AMPh (1·563 Å), but agrees well with similar bonds in other organic phosphates (Corbridge, 1974).

The P–C distance (1·808 Å) is comparable to the P–CH_2 distances in β-ciliatine (Okaya, 1966), β-AMPh (Darriet *et al.*, 1975), AMMPh (Głowiak & Sawka-Dobrowolska, 1977) and nitrilotris(methylenephosphonic acid) (Daly & Wheatley, 1967). The C(1)–C(2) and C(2)–C(3) distances (1·551 Å) are typical of values reported for such bonds.

There are four independent hydrogen bonds; three are of the type N–H···O and one is of the type O–H···O. The N atom makes three hydrogen bonds of the usual length, two to O(2) and one to O(3). A flattened tetrahedron is formed around the N atom by O(1), O(2), O(3) and C(3). The angles involving C(3) are smaller than the usual tetrahedral angle (94·40, 107·96, 108·96°); two of the three angles between hydrogen bonds are larger than ideal (115·27, 121·10°) and one is smaller (106·68°).

The N···O(2)($\frac{1}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} + z$), N···O(2)($-x$, $-y$, $\frac{1}{2} + z$), and N···O(3)(x, $y - 1$, z) distances are 2·812 (14), 2·811 (14) and 2·831 (13) Å respectively; the H(7)···O(2), H(8)···O(2) and H(9)···O(3) distances are 1·809, 1·820 and 1·873 Å. ∠N–H(7)···O(2) = 174·5 and ∠N–H(8)···O(2) = 168·9° are almost linear and ∠N–H(9)···O(3) = 154·8° is less so. Although the H atom of the O(1)–H group has not been determined, the distance O(1)···O(3)($\frac{1}{2} + x$, $\frac{1}{2} - y$, z) = 2·522 (12) Å strongly suggests the existence of an O–H···O hydrogen bond. The arrangement of the H atoms proves that 3-aminopropylphosphonic acid exists as a zwitterion, and thus the formula should be written $H_3^+N–(CH_2)_3–PO_3H^-$.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34924 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England

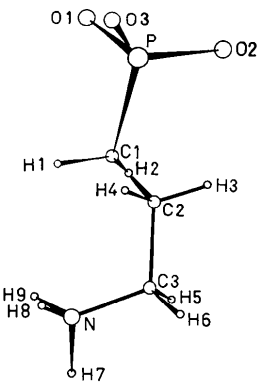

Fig. 1. Projection along the *a* axis of the molecule of 3-aminopropylphosphonic acid.

Table 2. *Bond distances* (Å) *and angles* (°)

P–O(1)	1·603 (9)	O(2)–P–O(1)	112·2 (5)
P–O(2)	1·505 (10)	O(3)–P–O(1)	104·3 (5)
P–O(3)	1·534 (9)	O(3)–P–O(2)	115·3 (5)
P–C(1)	1·808 (12)	C(1)–P–O(1)	105·0 (5)
C(1)–C(2)	1·551 (18)	C(1)–P–O(2)	108·4 (6)
C(2)–C(3)	1·551 (15)	C(1)–P–O(3)	111·1 (6)
C(3)–N	1·524 (21)	P–C(1)–C(2)	110·5 (8)
		C(1)–C(2)–C(3)	112·9 (10)
		C(2)–C(3)–N	112·3 (11)

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