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Benzenephosphonic Acid

BY T. J. R. WEAKLEY

Chemistry Department, Dundee University, Dundee DD1 4HN, Scotland

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Abstract. $C_6H_7O_3P$, *Pbca*; $a=11{\cdot}182$ (7), $b=8{\cdot}051$ (5), $c=15{\cdot}768$ (11) Å; $Z=8$, $D_m=1{\cdot}47$ (2), $D_x=1{\cdot}48$ g cm^{-3}; μ(Cu $K\alpha$)$=28{\cdot}7$ cm^{-1}. Puckered layers at $z=0$ and $z=\frac{1}{2}$ result from intermolecular hydrogen bonding. Only weak contacts occur between layers.

Introduction. Crystals were from a commercial sample (plates, prominent {001} faces). Equi-inclination multi-film Weissenberg photographs were recorded (Cu radiation, $\lambda=1{\cdot}5418$ Å) for the levels $h0$–$6l$, 0–$5kl$, and $hk0$–3; all crystals measured about $0{\cdot}3\times0{\cdot}3\times0{\cdot}05$ mm. Intensities were measured by a scanning microdensitometer (S.R.C. Service, Atlas Computer Laboratory). Absorption corrections were applied. Following a symbolic addition procedure, an E map showed the P and the adjacent C and three O atoms. A difference map phased by these gave the positions of the remaining C atoms. Refinement was by full-matrix least squares.

A second difference map, when R had fallen to 0·062, showed all H atoms near their expected positions; these were refined in subsequent cycles. The final unweighted R was 0·048 (anisotropic P, O, and C; isotropic H; 119 parameters, 768 independent reflexions

Table 1. *Atomic parameters*

Parameters for non-hydrogen atoms are multiplied by 10^4; those for hydrogen atoms, by 10^3. The thermal function is $T=\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{23}klb^*c^*)]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P	1583 (1)	484 (1)	699 (1)	332 (6)	278 (7)	494 (6)	4 (5)	−6 (5)	9 (5)
O(1)	1254 (3)	−1154 (5)	317 (2)	420 (18)	319 (20)	465 (20)	4 (16)	−120 (16)	−95 (17)
O(2)	811 (3)	1923 (5)	343 (2)	484 (17)	308 (19)	589 (20)	34 (18)	−129 (15)	52 (16)
O(3)	2896 (3)	927 (5)	516 (2)	381 (18)	367 (20)	764 (25)	−4 (15)	113 (16)	60 (20)
C(1)	1406 (4)	437 (5)	1816 (3)	380 (20)	304 (27)	538 (24)	74 (19)	−4 (18)	31 (24)
C(2)	407 (5)	−358 (8)	2165 (4)	466 (28)	562 (40)	620 (31)	−98 (27)	67 (24)	38 (29)
C(3)	223 (6)	−374 (9)	3036 (4)	753 (38)	646 (49)	702 (37)	8 (36)	226 (37)	117 (37)
C(4)	1039 (8)	365 (9)	3566 (4)	1056 (57)	685 (49)	486 (29)	249 (43)	2 (35)	129 (34)
C(5)	2016 (7)	1190 (9)	3233 (5)	876 (49)	678 (45)	650 (35)	48 (44)	−231 (35)	−21 (40)
C(6)	2210 (5)	1213 (8)	2357 (4)	541 (29)	537 (40)	588 (34)	−55 (28)	−146 (25)	6 (29)

	x	y	z	U		x	y	z	U
H(1)	316 (6)	215 (10)	48 (5)	80 (21)	H(5)	89 (9)	23 (11)	423 (7)	129 (31)
H(2)	−2 (7)	168 (11)	16 (5)	118 (31)	H(6)	286 (7)	167 (9)	351 (5)	108 (25)
H(3)	−20 (5)	−103 (8)	181 (4)	64 (16)	H(7)	304 (5)	175 (7)	209 (3)	53 (15)
H(4)	−58 (5)	−111 (9)	331 (4)	77 (19)					

Table 2. *Molecular dimensions and intermolecular distances*

P——O(1)	1·496 (4) Å	C(6)–C(1)	1·388 (7) Å
P——O(2)	1·550 (4)	O(2)–H(2)	0·99 (8)
P——O(3)	1·539 (3)	O(3)–H(1)	1·03 (8)
P——C(1)	1·773 (5)	C(2)–H(3)	1·03 (6)
C(1)–C(2)	1·400 (7)	C(3)–H(4)	1·16 (7)
C(2)–C(3)	1·389 (8)	C(4)–H(5)	1·06 (12)
C(3)–C(4)	1·374 (10)	C(5)–H(6)	1·11 (8)
C(4)–C(5)	1·382 (11)	C(6)–H(7)	1·11 (5)
C(5)–C(6)	1·398 (9)		

C(1)–P——O(1)	110·7 (2)°	O(1)–P——O(2)	112·1 (2)°
C(1)–P——O(2)	108·3 (2)	O(1)–P——O(3)	111·3 (2)
C(1)–P——O(3)	107·4 (2)	O(2)–P——O(3)	106·9 (2)

C–C–C 118·8 (6) to 120·7 (6)°

Hydrogen bonds

O(3)···O(1)^{i}	2·554 (6) Å	O(2)···O(1)^{ii}	2·608 (5) Å
O(3)–H(1)–O(1)^{i}	169 (12)°	O(2)–H(2)–O(1)^{ii}	169 (12)°

Other intermolecular distances

H(5)···O(3)^{iii}	2·61 (29) Å	C(4)···O(3)^{iii}	3·45 (3) Å
H(5)···O(2)^{iv}	2·88 (29)	C(4)···O(2)^{iv}	3·56 (3)
H(6)···O(1)^{iii}	3·04 (25)	C(5)···O(2)^{iv}	3·84 (3)
		C(6)···C(2)^{i}	3·85 (5)

Symmetry code

Superscript	x	y	z
None	x	y	z
i	$\frac{1}{2}-x$	$\frac{1}{2}+y$	z
ii	$-x$	$-y$	$-z$
iii	$\frac{1}{2}-x$	$-y$	$\frac{1}{2}+z$
iv	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$

above background). G. M. Sheldrick's *SHELX* program was used in all calculations. Positional and thermal parameters are listed in Table 1.*

Discussion. The dimensions of $C_6H_5PO(OH)_2$ and the bond angles at P (Table 2) are normal. Each OH oxygen atom participates in one near-linear hydrogen bond and the third O (shortest P–O bond) in two, as expected (Table 2). The hydrogen-bond network is of interest. For molecules of the type $XO(OH)_2$ three-dimensional nets, plane nets, or chains are possible

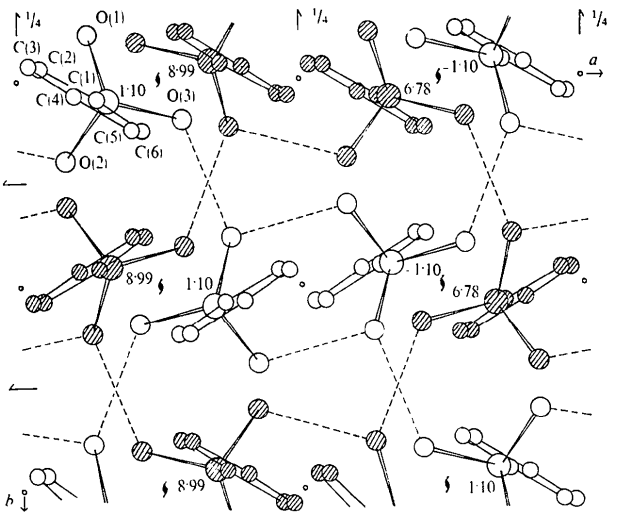

Fig. 1. A *c* axis projection; heights of P atoms (Å) are given. Open and shaded atoms are in layers centred at $z=0$ and $z=\frac{1}{2}$ respectively.

(Wells, 1975). Respective examples are $HPO(OH)_2$ (Furberg & Landmark, 1957); $SeO(OH)_2$ (Wells & Bailey, 1949); and $C_6H_5AsO(OH)_2$ (Shimada, 1960). In the present case, P has replaced As in $C_6H_5AsO(OH)_2$; the tetrahedral bonds are shortened by less than 0·2 Å, but this is accompanied by a change in molecular packing to give a double-layer structure (Fig. 1). The hydrogen-bonded layers, unlike those in $SeO(OH)_2$, include centrosymmetric pairs of molecules. Each pair is opposite large voids in the adjacent layers, and the phenyl groups project towards these voids. The weak forces between layers (Table 2) are reflected in the crystal habit and the ready cleavage normal to **c**.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31827 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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