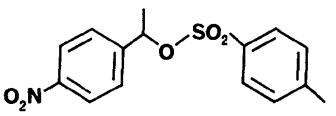
atoms anisotropic; H atoms included using riding model with C–H 0·96 Å, H–C–H 109·5°, U(H) = 1·2U_{eq}(C); weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}00025F^2$; 204 parameters; $S = 1{\cdot}80$; max. Δ/σ 0·02; max. and min. features in final $\Delta\rho$ map 0·7, −0·5 e Å^{-3}. Absolute structure (Jones, 1984) weakly indicated by η refinement (Rogers, 1981); $\eta = 1{\cdot}3$ (3). Atomic scattering factors from *SHELXTL*. Final atomic coordinates are given in Table 1, and bond lengths and angles in Table 2.* Fig. 1 shows the atom-numbering scheme.

Related literature. For results of a series of structure determinations of ethers and esters of 1-(4-nitrophenyl)ethanol, see Jones, Edwards & Kirby (1986). The large difference peak near the C–O–S moiety, possibly an unidentified minor disorder or twinning phenomenon, precludes the comparison of the current structure (1).



(1)

* Lists of structure factors, H-atom coordinates, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43068 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

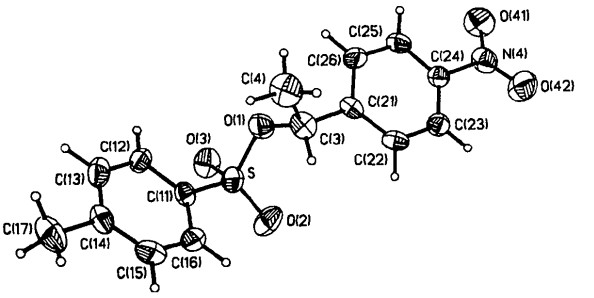


Fig. 1. Molecule of the title compound, showing the atom-numbering scheme.

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Bis(cyclohexylammonium) Hydrogenphosphate

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Abstract. $2C_6H_{14}N^+.HPO_4^{2-}$, $M_r = 296{\cdot}35$, monoclinic, $P2_1/c$, $a = 14{\cdot}451$ (4), $b = 12{\cdot}955$ (4), $c = 8{\cdot}157$ (2) Å, $\beta = 90{\cdot}11$ (2)°, $U = 1527{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}29$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2{\cdot}0$ cm^{-1}, $F(000) = 648$, $T = 293$ K, $R = 0{\cdot}044$ for 2265 reflections. A hydrogen-bonding network connects NH_3^+ and HPO_4^{2-} units and also the phosphate ions amongst themselves; all X–H atoms (X = O or N) are donors and all O atoms (except that bearing H) twofold acceptors. P–O bond lengths 1·609 (2) to (OH), 1·510 (2), 1·514 (2), 1·522 (2) Å.

Experimental. Stoe two-circle diffractometer, monochromated Mo $K\alpha$ radiation, $2\theta_{max}$ 50°, two crystals: (*a*) colourless needle, 0·55 × 0·1 × 0·1 mm, mounted about **b**, layers 0–14, 5034 reflections, and (*b*) 0·7 × 0·2 × 0·1 mm, mounted about **c** (the needle axis), layers 0–2, 1259 reflections. No absorption correction. Interlayer scale factors by analysis of common reflections. 2806 unique reflections (R_{int} 0·023), 2265 with $F > 4\sigma(F)$ used for all calculations (program system *SHELXTL*; Sheldrick, 1983). Index range after merging: $|h| \le 17$, $k \le 15$, $l \le 9$. Cell constants refined from $\pm 2\theta$ values of 22 reflections [measured on Stoe–Siemens four-circle diffractometer with crystal (*b*)].

Structure solution by routine direct methods, four missing non-H atoms located in difference synthesis.

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Table 1. *Atom coordinates* ($\times 10^4$) *and isotropic temperature factors* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}*
P	113 (1)	1422 (1)	7240 (1)	21 (1)
O(1)	653 (1)	1438 (1)	5518 (2)	30 (1)
O(2)	687 (1)	688 (1)	8260 (2)	31 (1)
O(3)	116 (1)	2520 (1)	7903 (2)	31 (1)
O(4)	−854 (1)	1018 (1)	6921 (2)	31 (1)
N(1)	1211 (1)	−980 (1)	6443 (2)	24 (1)
C(11)	2209 (1)	−1183 (1)	6732 (2)	23 (1)
C(12)	2778 (1)	−241 (1)	6255 (3)	29 (1)
C(13)	3809 (1)	−451 (2)	6516 (3)	40 (1)
C(14)	4121 (1)	−1406 (2)	5589 (3)	42 (1)
C(15)	3536 (1)	−2340 (2)	6030 (3)	39 (1)
C(16)	2505 (1)	−2137 (1)	5790 (3)	32 (1)
N(2)	1164 (1)	859 (1)	1491 (2)	24 (1)
C(21)	2169 (1)	1085 (1)	1752 (2)	23 (1)
C(22)	2453 (1)	2047 (1)	807 (3)	34 (1)
C(23)	3478 (1)	2269 (2)	1049 (3)	38 (1)
C(24)	4078 (1)	1354 (2)	604 (3)	40 (1)
C(25)	3781 (1)	393 (2)	1532 (3)	40 (1)
C(26)	2753 (1)	165 (1)	1276 (3)	30 (1)

* Equivalent isotropic U calculated from anisotropic U.

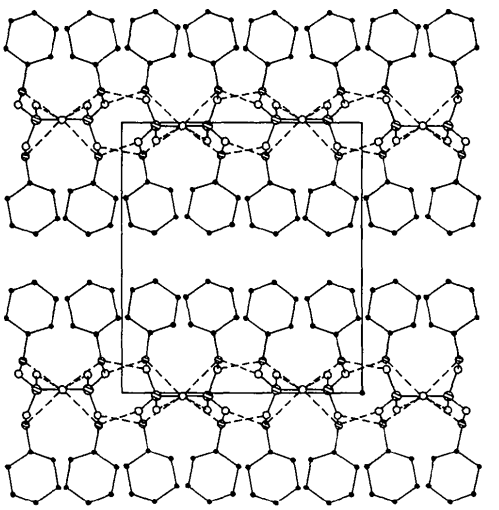

Fig. 1. Packing plot projected down **b**. The origin is indicated by a black dot. Atom key: hatched atoms P (large), N (small), open circles O, filled circles C. H bonds are indicated by broken lines.

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

O(1)–P	1·609 (2)	O(2)–P	1·510 (2)
O(3)–P	1·522 (2)	O(4)–P	1·514 (2)
C(11)–N(1)	1·485 (3)	C(11)–C(12)	1·522 (4)
C(11)–C(16)	1·517 (4)	C(12)–C(13)	1·528 (4)
C(13)–C(14)	1·519 (4)	C(14)–C(15)	1·519 (4)
C(15)–C(16)	1·525 (4)	C(21)–N(2)	1·495 (3)
C(21)–C(22)	1·521 (4)	C(21)–C(26)	1·513 (4)
C(22)–C(23)	1·522 (4)	C(23)–C(24)	1·513 (4)
C(24)–C(25)	1·519 (4)	C(25)–C(26)	1·529 (4)
O(1)–H	0·87 (3)		

O(1)–P–O(2)	102·8 (2)	O(1)–P–O(3)	107·3 (2)
O(2)–P–O(3)	113·0 (2)	O(1)–P–O(4)	107·7 (2)
O(2)–P–O(4)	112·5 (2)	O(3)–P–O(4)	112·7 (2)
N(1)–C(11)–C(12)	110·1 (2)	N(1)–C(11)–C(16)	109·8 (3)
C(12)–C(11)–C(16)	111·7 (3)	C(11)–C(12)–C(13)	110·4 (3)
C(12)–C(13)–C(14)	111·5 (3)	C(13)–C(14)–C(15)	111·4 (3)
C(14)–C(15)–C(16)	112·1 (3)	C(11)–C(16)–C(15)	110·6 (3)
N(2)–C(21)–C(22)	110·6 (3)	N(2)–C(21)–C(26)	110·6 (2)
C(22)–C(21)–C(26)	111·4 (3)	C(21)–C(22)–C(23)	110·7 (3)
C(22)–C(23)–C(24)	112·2 (3)	C(23)–C(24)–C(25)	111·1 (3)
C(24)–C(25)–C(26)	111·5 (3)	C(21)–C(26)–C(25)	110·8 (3)
P–O(1)–H	119 (2)		

Table 3. *Hydrogen bonding*

X–H···Y	X···Y (Å)	H···Y (Å)	Y at
O(1)–H···O(3)	2·64	1·80	$x, 0·5-y, -0·5+z$
N(2)–H(2*c*)···O(2)	2·73	1·77	$x, y, -1+z$
N(1)–H(1*c*)···O(2)	2·73	1·77	x, y, z
N(1)–H(1*a*)···O(3)	2·78	1·86	$-x, -0·5+y, 1·5-z$
N(2)–H(2*b*)···O(4)	2·79	1·83	$-x, -y, 1-z$
N(1)–H(1*b*)···O(4)	2·79	1·85	$-x, -y, 1-z$
N(2)–H(2*a*)···O(3)	2·84	1·88	$x, 0·5-y, -0·5+z$

Refinement on F to R 0·044, wR 0·052. All non-H atoms anisotropic; phosphate acidic H freely refined, all other H included using riding model with C–H and N–H 0·96 Å, H–C–H and H–N–H 109·5°, U(H) $= 1·2U_{eq}$(C or N); weighting scheme $w^{-1} = \sigma^2(F) + 0·0005F^2$; 182 parameters; $S = 1·57$; max. Δ/σ 0·009; max. features in final $\Delta\rho$ map 0·4 (near P), −0·3 e Å^{-3}. Atomic scattering factors from *SHELXTL*. Final atomic coordinates are given in Table 1, bond lengths and angles in Table 2, and H-bond distances in Table 3.* Fig. 1 shows the molecular packing.

Related literature. The compound was prepared during a study of organic phosphate dianions (Jones, Sheldrick, Kirby & Abell, 1984*a*,*b*). For a summary of phosphate structures see Wells (1984).

I thank Dr A. J. Kirby and Mrs K. W. Y. Abell for providing the sample and the Verband der Chemischen Industrie for financial support.

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