Table 3. *Deviations* ($\times 10^3$ Å) *of atoms from the plane of the benzene ring*

C(1)*	1	C(6)*	2
C(2)*	−2	C(7)	18
C(3)*	1	C(8)	121
C(4)*	2	O	−27
C(5)*	−3		

* The atoms used for the calculation of the least-squares plane.

All the calculations were performed on the FACOM 270-30 of this Institute with a local version of the Universal Crystallographic Computation Program System UNICS (Crystallographic Society of Japan, 1967). Part of the cost of this research was met by a Scientific Research Grant from the Ministry of Education to which the authors' thanks are due.

Table 4. *Intermolecular contacts with their standard deviations in parentheses*

(*a*) Between non-hydrogen atoms

$C(5^{i})\cdots O^{ii}$	3·379 (2) Å

(*b*) Between hydrogen and other atoms

$H(4^{i})\cdots O^{ii}$	2·69 (2)
$H(5^{i})\cdots C(2^{ii})$	3·02 (2)
$H(5^{i})\cdots C(7^{ii})$	3·02 (2)
$H(2^{i})\cdots H(3^{iii})$	2·54 (3)
$H(2^{i})\cdots C(5^{iii})$	3·08 (3)
$H(2^{i})\cdots H(4^{iii})$	2·53 (3)
$O^{i}\cdots\cdots H(8^{iv})$	2·48 (2)
$H(1^{i})\cdots C(5^{iv})$	2·97 (1)

Superscripts indicate the following equivalent positions:

i	x	y	z
ii	$0{\cdot}5-x$	$0{\cdot}5+y$	$0{\cdot}5-z$
iii	$0{\cdot}5-x$	$-0{\cdot}5+y$	$1{\cdot}5-z$
iv	$0{\cdot}5+x$	$1{\cdot}5-y$	$0{\cdot}5+z$

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The Crystal Structure of Dimethyl Ammonium Phosphate, $NH_4(CH_3)_2PO_4$

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(*Received* 12 *March* 1973; *accepted* 14 *March* 1973)

$NH_4(CH_3)_2PO_4$ is monoclinic, space group $P2_1/c$, with $a=10{\cdot}20$ (1), $b=6{\cdot}88$ (1), $c=9{\cdot}74$ (1) Å, $\beta=105{\cdot}5$ (3)° and $Z=4$. The structure was determined from intensities measured on a two-circle diffractometer by Patterson and Fourier syntheses, and refined by the least-squares method (667 observed reflexions). The final R value, without contributions from the hydrogen atoms, is 0·076. Due to the existence of hydrophobic and hydrophilic parts in the molecule, a layer structure is present, extending parallel to the bc plane.

Introduction

The need for accurate structural investigations of alkyl-phosphates was emphasized by Cruickshank (1961). Recently, Hazel & Collin (1972) detailed the importance of phosphate diesters and their implications regarding the structure of nucleic acids. A structural analysis of dimethyl ammonium phosphate, $NH_4(CH_3)_2PO_4$, can contribute by providing information about the angles of internal rotation about the C–O bond. In addition, the recent publication of structures of diammonium hydrogen phosphate $(NH_4)_2HPO_4$ (Khan, Roux & James, 1972), and of methyl diammonium phosphate dihydrate $(NH_4)_2CH_3PO_4.2H_2O$ (Garbassi, Giarda & Fagherazzi, 1972), reveals a continued interest in ammonium phosphates.

Experimental

In the reaction between P_2O_5, ammonia and methanol in chloroform, a mixture of various ammonium methyl phosphates is obtained (Gilli & Zani, 1973). The two major components of the reaction product are diammonium methyl phosphate, whose structure in the dihydrate form has already been determined (Garbassi, Giarda & Fagherazzi, 1972), and dimethyl ammonium phosphate. The latter can be easily separated in ethanol and recrystallized. Colourless, elongated plates are obtained. X-ray data were taken on a crystal with transversal dimensions about 0·2×0·15 mm, around the *c* axis. Weissenberg photographs showed the space group extinctions $k=2n+1$ for $0k0$ and $l=2n+1$ for $h0l$; the space group is therefore $P2_1/c$.

Crystal data are: $a=10{\cdot}20\,(1)$, $b=6{\cdot}88\,(1)$, $c=9{\cdot}74\,(1)$ Å, $\beta=105{\cdot}5\,(3)°$, $V=658{\cdot}7$ Å^3, $Z=4$, $D_{\rm obs}=1{\cdot}433$, $D_{\rm calc}=1{\cdot}440$ g cm^{-3}, M.W. 143·08.

The intensity data were collected on a Stoe automatic diffractometer by the equi-inclination technique, using Cu $K\alpha$ radiation. The θ–2θ scanning mode was used, and the scan speed (between 0·5 and 4°/min) and the attenuation filters were automatically selected according to the reflexion intensities. Stationary crystal and counter background counts for 1 min were taken at each end of the scan, whose width, $\Delta\theta$, was 2·5°. The measurements were made up to $2\theta=130°$. Six independent reflexions, with their symmetry equivalents, were assumed as standards and monitored between each layer collection. Good stability was found. 743 reflexions were measured, and 667 of them, having an intensity higher than 2·5 times the calculated standard deviation, were considered observed.

Background, attenuation and Lorentz–polarization corrections were made by means of the program furnished by Stoe. No correction was considered necessary for absorption, since μR was about 0·6.

Determination and refinement of the structure

A three-dimensional Patterson synthesis revealed the P–P vector. The remaining non-hydrogen atoms were located by electron density syntheses. At this stage, a structure factor calculation, with atomic scattering factors calculated following Moore (1963), gave $R=0{\cdot}33$. The full-matrix least-squares refinement was

Table 1. *Observed and calculated structure factors*

Unobserved *F*'s are marked by an <. Zero weight *F*'s in the least-squares refinement are indicated by an *E*.

H	K	L		FO	FC
1	0	0		170	174
2	0	0	E	387	-413
3	0	0		30	-51
4	0	0		78	73
5	0	0		248	252
6	0	0		102	-104
7	0	0		199	-201
8	0	0		59	56
9	0	0		120	122
10	0	0		40	62
1	1	0	E	317	-375
11	0	0		73	-73
2	1	0	<	0	-5
3	1	0		52	-73
4	1	0		173	164
5	1	0		69	57
6	1	0		99	-89
7	1	0		135	144
8	1	0		174	174
9	1	0		11	-7
10	1	0		40	-38
11	1	0		33	-34
0	2	0		61	-47
1	2	0		62	-34
2	2	0		229	-218
3	2	0		135	-120
4	2	0		188	185
5	2	0		92	85
6	2	0	<	0	0
7	2	0		30	-26
8	2	0		63	-62
9	2	0		13	14
10	2	0		14	14
11	2	0		18	-19
1	3	0		16	-16
2	3	0		65	-56
3	3	0		157	146
4	3	0		157	155
5	3	0		121	-118
6	3	0		101	-102
7	3	0	<	0	4
8	3	0		35	30
9	3	0		23	23
10	3	0		43	-42
0	4	0		70	-68
1	4	0	<	0	0
2	4	0		64	64
3	4	0	<	0	8
4	4	0		183	-135
5	4	0		83	-73
6	4	0		56	55
7	4	0		28	26
8	4	0		16	14
9	4	0		36	-36
10	4	0	<	0	-9
1	5	0		62	55
2	5	0		12	5
3	5	0		111	-113
4	5	0		90	-84
5	5	0		58	54
6	5	0		31	30
7	5	0		28	-26
8	5	0		47	-49
9	5	0		21	-19
0	6	0		20	17
1	6	0		49	49
2	6	0		23	-29
3	6	0	<	0	5
4	6	0		55	55
5	6	0		40	40
6	6	0	<	0	-4
7	6	0	<	0	-6
1	7	0		50	51
2	7	0	<	0	3
3	7	0		9	-4
4	7	0		9	-9
5	7	0		32	32
0	8	0		51	56
1	8	0	<	0	-6
0	1	1		206	232
1	1	1		177	-187
2	1	1		341	-358
3	1	1		149	139
4	1	1		250	253
5	1	1		19	11
6	1	1		108	-96
7	1	1		54	-55
8	1	1		74	68
9	1	1		59	63
10	1	1		17	-15
11	1	1		29	-33
0	2	1		173	-171
1	2	1		175	-185
2	2	1		75	-66
3	2	1		117	132
4	2	1		27	-21
5	2	1		181	-184
6	2	1		119	-125
7	2	1		85	87
8	2	1		74	72
9	2	1		56	-58
10	2	1		32	-37
0	3	1		45	38
1	3	1		83	67
2	3	1		32	21
3	3	1		79	-76
4	3	1		95	-100
5	3	1		23	-31
6	3	1		61	54
7	3	1	<	0	7
8	3	1		67	-65
9	3	1		20	-21
10	3	1		9	8
0	4	1		114	106
1	4	1		28	-26
2	4	1		96	-92
3	4	1		60	57
4	4	1		94	89
5	4	1		72	71
6	4	1	<	0	9
7	4	1		21	-20
8	4	1		26	27
9	4	1	<	0	1
0	5	1		77	-75
1	5	1		41	-41
2	5	1		115	118
3	5	1	<	0	-1
4	5	1		31	-30
5	5	1		56	56
6	5	1	<	0	4
7	5	1	<	0	8
8	5	1		26	-23
0	6	1		92	88
1	6	1		88	85
2	6	1		47	-45
3	6	1		101	-99
4	6	1		66	66
5	6	1		48	47
6	6	1		27	-30
7	6	1		59	-62
0	7	1		29	30
1	7	1		37	-40
2	7	1		85	-84
3	7	1		22	24
4	7	1		53	58
5	7	1		17	-18
0	8	1		14	-16
1	8	1		56	-59
-1	1	1		193	221
-2	1	1		223	-213
-3	1	1		295	-314
-4	1	1		14	-7
-5	1	1		134	134
-6	1	1		85	88
-7	1	1		125	-126
-8	1	1		111	-114
-9	1	1		63	61
-10	1	1		53	51
-11	1	1		18	-20
-1	2	1		44	19
-2	2	1		214	207
-3	2	1		199	-182
-4	2	1		229	-230
-5	2	1		19	18
-6	2	1		158	154
-7	2	1		90	90
-8	2	1		95	-80
-9	2	1		29	-28
-10	2	1		61	60
-11	2	1		47	49
-1	3	1		83	40
-2	3	1		179	164
-3	3	1		81	89
-4	3	1		8	-7
-5	3	1	<	11	-5
-6	3	1		27	-22
-7	3	1		80	76
-8	3	1		58	54
-9	3	1		20	-18
-10	3	1	<	0	-5
-1	4	1		31	29
-2	4	1		62	57
-3	4	1		23	15
-4	4	1	<	0	-4
-5	4	1		89	87
-6	4	1		21	-29
-7	4	1		74	-73
-8	4	1		17	-11
-9	4	1		14	-17
-10	4	1	<	0	1
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-2	5	1		31	-29
-3	5	1		44	45
-4	5	1		43	-47
-5	5	1		27	-21
-6	5	1		22	23
-7	5	1		17	14
-8	5	1		17	20
-9	5	1		44	-49
-1	6	1		25	25
-2	6	1		140	-144
-3	6	1		45	-46
-4	6	1		92	89
-5	6	1		10	11
-6	6	1		44	-40
-7	6	1		30	-29
-1	7	1		82	87
-2	7	1		19	18
-3	7	1		92	-96
-4	7	1		24	-24
-5	7	1		29	31
-6	7	1	<	0	1
-1	8	1	<	0	7
1	0	2	E	318	-420
2	0	2		162	-128
3	0	2		125	-117
4	0	2		80	71
5	0	2		135	-142
6	0	2		137	-132
7	0	2		134	129
8	0	2		44	40
9	0	2		23	-22
10	0	2		45	-48
0	1	2	E	318	-362
1	1	2		104	115
2	1	2		43	43
3	1	2		97	99
4	1	2		105	98
5	1	2		102	-105
6	1	2		79	83
7	1	2		60	59
8	1	2		69	-72
9	1	2		59	-62
10	1	2		39	-44
0	2	2		102	93
1	2	2		98	100
2	2	2		64	64
3	2	2		172	161
4	2	2		13	-5
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6	2	2		34	36
7	2	2		54	-53
8	2	2		13	-14
9	2	2	<	0	12
10	2	2		9	10
0	3	2		29	-33
1	3	2		47	-50
2	3	2		93	94
3	3	2		41	34
4	3	2		64	-58
5	3	2		76	-78
6	3	2		37	-35
7	3	2		49	52
8	3	2		38	38
9	3	2		35	-36
10	3	2	<	0	1
0	4	2		59	-47
1	4	2		152	150
2	4	2		47	49
3	4	2		150	-141
4	4	2		57	-60
5	4	2		110	107
6	4	2		91	89
7	4	2	<	0	-9
8	4	2		47	-47
9	4	2	<	0	4
0	5	2		55	48
1	5	2		83	-90
2	5	2		169	-163
3	5	2	<	0	9
4	5	2		136	139
5	5	2		30	32
6	5	2		65	-63
7	5	2		29	-32
8	5	2		27	28
0	6	2		39	-36
1	6	2		44	-48
2	6	2	<	0	-6
3	6	2		31	36
4	6	2		24	-23
5	6	2		44	-47
6	6	2		20	-22
0	7	2		74	73
1	7	2		40	-41
2	7	2		31	-31
3	7	2		26	27
4	7	2		32	33
-3	0	2		67	54
-4	0	2		76	-70
-5	0	2		20	-10
-6	0	2		174	184
-7	0	2		37	-40
-8	0	2		132	-139
-9	0	2		35	41
-10	0	2		112	111
-11	0	2		47	51
-1	1	2		19	8
-2	1	2		307	350
-3	1	2		127	93
-4	1	2		89	90
-5	1	2		41	33
-6	1	2		78	74
-7	1	2		103	105
-8	1	2		49	-49
-9	1	2		93	-91
-10	1	2		15	-16
-11	1	2		27	25
-1	2	2		189	-198
-2	2	2		48	-33
-3	2	2		16	-14
-4	2	2		113	-104
-5	2	2		67	61
-6	2	2		25	19
-7	2	2	<	0	-6
-8	2	2		33	35
-9	2	2		24	-28
-10	2	2		21	-23
-11	2	2		17	-16
-1	3	2		140	128
-2	3	2		80	80
-3	3	2	<	0	-2
-4	3	2		186	-181
-5	3	2		89	-86
-6	3	2		112	111
-7	3	2	<	0	7
-8	3	2	<	0	0
-9	3	2	<	0	-4
-10	3	2		14	-19
-11	3	2		48	52
-1	4	2		55	-56
-2	4	2		9	9
-3	4	2		86	82
-4	4	2		150	135
-5	4	2		111	-109
-6	4	2		130	-125
-7	4	2	<	0	12
-8	4	2		33	35
-9	4	2		22	22
-10	4	2		64	-64
-1	5	2		53	50
-2	5	2		66	-61
-3	5	2		173	-180
-4	5	2		22	20
-5	5	2		123	127
-6	5	2		27	-27
-7	5	2		68	-66
-8	5	2		46	-40
-9	5	2		31	27
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-2	6	2		41	44
-3	6	2		26	-19
-4	6	2		42	-39
-5	6	2		25	25
-6	6	2		25	23
-7	6	2		36	37
-8	6	2		19	17
-1	7	2		67	67
-2	7	2		10	-11
-3	7	2		24	-24
-4	7	2		15	14
-5	7	2		51	51
-6	7	2		9	8
0	1	3		100	72
1	1	3		157	148
2	1	3		50	58
3	1	3		60	63
4	1	3		46	-39
5	1	3		47	-33
6	1	3		30	31
7	1	3		36	34
8	1	3		14	-12
9	1	3		36	-36
10	1	3	<	0	-2
0	2	3		24	-39
1	2	3		110	109
2	2	3		125	131
3	2	3		52	-50
4	2	3		83	-89
5	2	3		49	45
6	2	3		99	101
7	2	3		50	52
8	2	3		34	-35
9	2	3		19	-19
10	2	3		38	44
0	3	3		86	79
1	3	3		27	28
2	3	3		128	-130
3	3	3		191	-203
4	3	3	<	0	-7
5	3	3		131	140
6	3	3		31	33
7	3	3		74	-77
8	3	3		27	-31
9	3	3		42	42
0	4	3		50	-55
1	4	3		80	-92
2	4	3	<	0	10
3	4	3		25	21
4	4	3		56	52
5	4	3		17	-15
6	4	3		76	-80
7	4	3	<	0	-13
8	4	3	<	0	-2
0	5	3		42	42
1	5	3		124	124
2	5	3		19	22
3	5	3		67	-64
4	5	3		29	29
5	5	3		22	22
6	5	3	<	0	-1
7	5	3		35	-35
0	6	3		41	47
1	6	3		81	-87
2	6	3		96	-98
3	6	3		74	71
4	6	3		52	56
5	6	3		48	-49
6	6	3		41	-48
0	7	3		55	-60
1	7	3		63	-62
2	7	3		54	56
3	7	3		61	66
4	7	3		35	-39
-1	1	3		119	-103
-2	1	3		73	80
-3	1	3		55	52
-4	1	3	<	0	-2
-5	1	3		10	-9
-6	1	3		22	24
-7	1	3		54	53
-8	1	3		41	-38
-9	1	3		28	-25
-10	1	3		11	12
-11	1	3	<	0	7
-1	2	3		185	-166
-2	2	3		125	112
-3	2	3		117	112
-4	2	3		161	-167
-5	2	3		100	-116
-6	2	3		105	-102
-7	2	3		35	30
-8	2	3		60	62
-9	2	3		64	-68
-10	2	3		47	-52
-11	2	3	<	0	4
-1	3	3		140	-143
-2	3	3		229	-239
-3	3	3		52	51
-4	3	3		112	117
-5	3	3		47	42
-6	3	3		115	-117
-7	3	3		127	-127
-8	3	3		70	73
-9	3	3		66	67
-10	3	3	<	0	-10
-11	3	3		20	-21
-1	4	3		77	75
-2	4	3		12	15
-3	4	3		31	-24
-4	4	3		14	-7
-5	4	3		74	73
-6	4	3		111	113
-7	4	3	<	0	1
-8	4	3		25	-22
-9	4	3	<	0	-1
-10	4	3		8	7
-1	5	3		11	11
-2	5	3		77	-80
-3	5	3		25	-37
-4	5	3		118	98
-5	5	3		18	11
-6	5	3		46	-44
-7	5	3	<	0	-6
-8	5	3		40	42
-9	5	3		28	30
-1	6	3		125	130
-2	6	3		47	49
-3	6	3		120	-125
-4	6	3		55	-55
-5	6	3		56	59
-6	6	3		36	34
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9	0	4		19	-21
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0	6	4		26	-23
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3	7	4		8	8
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3	1	5		110	-94
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2	4	5		33	-33
3	4	5		14	22
4	4	5		35	31
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-2	4	5		18	-27
-3	4	5		113	-110
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-9	4	5	<	0	-10
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-5	5	5		45	47
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-9	5	5		15	14
-1	6	5		33	41
-2	6	5		72	72
-3	6	5		20	20
-4	6	5		42	-49
-5	6	5		32	-32
-6	6	5		36	43
-7	6	5		22	28
-1	7	5		55	-56
-2	7	5		11	-7
-3	7	5		42	48
-4	7	5		35	33

Table 2. *Fractional atomic parameters* ($\times 10^4$) *and anisotropic thermal parameters* B_{ij} ($\times 10^2$) *with their standard deviations*

Temperature factor $= \exp\left[-\frac{1}{4}(B_{11}a^{*2}h^2 + B_{22}b^{*2}k^2 + B_{33}c^{*2}l^2 + 2B_{12}a^*b^*hk + 2B_{13}a^*c^*hl + 2B_{23}b^*c^*kl)\right]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
P	2219 (1)	1320 (2)	1407 (2)	234 (6)	163 (6)	177 (21)	−17 (4)	39 (7)	−10 (6)
O(1)	2131 (4)	511 (6)	−92 (7)	352 (20)	266 (19)	369 (48)	72 (16)	3 (21)	−84 (23)
O(2)	3687 (4)	2251 (6)	1931 (6)	261 (17)	313 (19)	178 (45)	−67 (14)	30 (19)	54 (18)
O(3)	1135 (4)	2835 (7)	1158 (7)	290 (19)	309 (20)	424 (20)	69 (15)	55 (20)	−56 (21)
O(4)	2183 (5)	−251 (7)	2464 (7)	557 (25)	325 (20)	180 (45)	−159 (19)	91 (22)	52 (21)
C(1)	3107 (10)	−932 (15)	−369 (16)	562 (48)	534 (47)	1282 (118)	285 (40)	68 (53)	−350 (58)
C(2)	4012 (9)	3840 (12)	1141 (13)	444 (38)	595 (36)	835 (93)	−182 (30)	132 (41)	136 (40)
N	358 (5)	6673 (7)	1678 (8)	324 (22)	229 (19)	234 (53)	−3 (17)	93 (23)	−33 (22)
Hydrogen atoms located by means of a difference Fourier map									
H(1)	−125	6910	256						
H(2)	750	5750	1440						

carried out with a program by Immirzi (1967), applying the weighting scheme suggested by Cruickshank (1965). Convergence was obtained with $R = 0{\cdot}12$.

The introduction of anisotropic thermal factors lowered R to 0·085, and the elimination of four low-angle reflexions probably suffering from extinction, gave a final R of 0·076 (0·080 including non-observed reflexions). An attempt to locate the hydrogen atoms from a difference map met with only partial success: two hydrogen atoms around nitrogen were located with certainty.

Table 1 lists observed and calculated structure factors. Final positional and thermal parameters with their standard deviations are given in Table 2.

Discussion

The dimethyl phosphate group

Bond distances and angles of the $(CH_3)_2O_2PO_2^-$ ion are listed in Table 3.

Table 3. *Interatomic distances and bond angles*

P–O(1)	1·536 (7) Å	O(1)–P–O(2)	104·8 (1)°
P–O(2)	1·582 (5)	O(1)–P–O(3)	104·5 (2)
P–O(3)	1·490 (5)	O(1)–P–O(4)	112·5 (2)
P–O(4)	1·498 (7)	O(2)–P–O(3)	111·4 (2)
Average	1·521	O(2)–P–O(4)	105·7 (2)
		O(3)–P–O(4)	117·2 (2)
O(1)–C(1)	1·481 (11)	Average	109·3
O(2)–C(2)	1·425 (12)		
Average	1·453	P–O(1)–C(1)	123·0 (4)
		P–O(2)–C(2)	118·3 (4)
N—H(1)	1·02	Average	120·6
N—H(2)	0·83		
O(1)–O(2)	2·478 (8)		
O(1)–O(3)	2·398 (6)		
O(1)–O(4)	2·532 (9)		
O(2)–O(3)	2·540 (7)		
O(2)–O(4)	2·455 (7)		
O(3)–O(4)	2·555 (8)		

In the PO_4 group there are two longer P–O bonds, where oxygen atoms are bonded to methyl groups, with an average value of 1·559 Å, and two shorter (average value: 1·494 Å). The PO_4 tetrahedron is slightly distorted with O–P–O angles between 104·5 and 112·5°. Only the angle between the two shorter P–O bonds (117·2°) is considerably greater than that of a regular tetrahedron, in agreement with the value generally accepted for unprotonated O–P–O angles (Karle & Britts, 1966).

There are few examples of structural refinements of phosphate diesters. A comparison of the P–OC bond lengths in these compounds is given in Table 4.

The lengths of PO–C bonds are generally near 1·43 Å (Sundaralingam & Putkey, 1970), but longer bonds are found, such as 1·502 Å in dipotassium ethyl phosphate tetrahydrate (McDonald & Cruickshank, 1971). Therefore, the bond lengths found by us, 1·425 and 1·481 Å, can be considered normal.

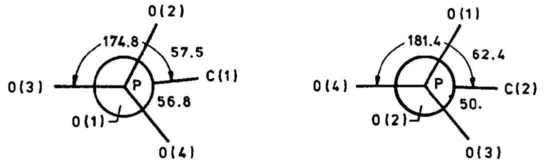

Fig. 1. Newman projections of the phosphate group along the P–OC bonds.

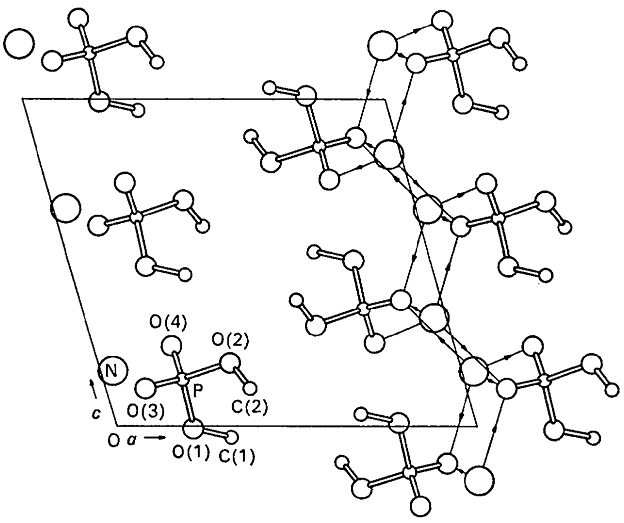

Fig. 2. Projection of the crystal structure along the *b* axis. The hydrogen bonds are indicated by arrows.

Table 4. P–OC *bond lengths in some phosphate diesters*

Dimethyl ammonium phosphate	1·582 (5) Å	1·536 (7) Å	This work
Dibenzylphosphoric acid	1·566	1·545	Dunitz & Rollett (1956)
Barium diethyl phosphate	1·62 (2)	1·59 (2)	Kyogoku & Iitaka (1966)
Silver diethyl phosphate	1·549 (8)	1·548 (9)	Hazel & Collin (1972)

Fig. 1 shows the Newman projections of the phosphate group along the P–OC bonds. The methyl group assumes in both cases a staggered conformation with respect to other oxygen atoms. A comparison between the angles of internal rotation around the P–OC bonds in phosphate diesters and in some polynucleotides was carried out by Kyogoku & Iitaka (1966). The values obtained in the present work, of ±57·5° (in mutually enantiomorphous molecules) for O(2)–P–O(1)–C(1) and ±62·4° for O(1)–P–O(2)–C(2) are in agreement with those obtained by the above authors in barium diethyl phosphate.

Examining the chains C–C–O–P–O–C–C in the latter compound, in dibenzylphosphoric acid (Dunitz & Rollett, 1956) and in silver diethyl phosphate (Hazel & Collin, 1972), the conformations of internal rotation angles are respectively: *trans*, *gauche*, *gauche*, *trans*; *trans*, *gauche*, *trans*, *trans*; *trans*, *gauche*, *skew*, *trans*. These results can be compared with a conformation *gauche*, *gauche* for the chain C–O–P–O–C in dimethyl ammonium phosphate.

Hydrogen bonding and packing of the molecules

Table 5 lists distances and angles of the coordination polyhedron around the NH_4^+ ion. Of the five nearest oxygen atoms, four, with distances varying from 2·79 to 3·03 Å (average value 2·86 Å) and placed at the corners of a distorted tetrahedron, can be accepted as hydrogen bonds. The N–H···O distances and the coordination number of nitrogen are in good agreement with those of several ammonium phosphates listed by Khan & Baur (1972). Only oxygen atoms not attached to methyl groups participate in the hydrogen bond system. Each O(3) acts three times as an acceptor, while O(4) is linked to the ammonium ion by only one hydrogen bond. In Fig. 3, the network of hydrogen bonds is shown in a projection on to the *bc* plane. For clarity, the atoms not involved are omitted. The grid is made up horizontally of ···O(3)···N···O(3)··· sequences and vertically of ···N···O(3)–P–O(4)··· N··· sequences. As shown in Fig. 2, the structure consist of double layers extending parallel to the *bc* plane. The layers are separated from each other by van der Waals contacts between the hydrophobic methyl groups. A similar situation can be found in aminoacid structures, such as L-valine (Torii & Iitaka, 1970) and L-isoleucine (Khawas, 1970).

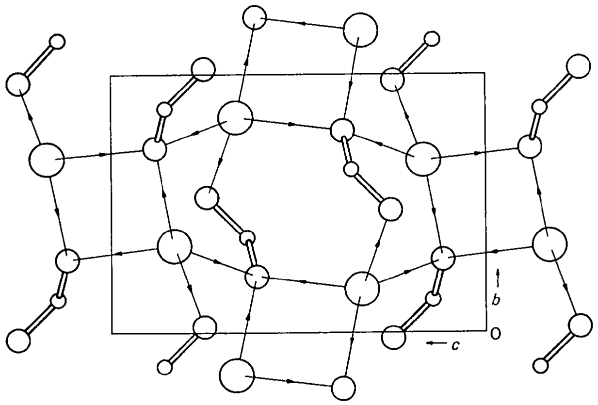

Fig. 3. The network of hydrogen bonds along the *a* axis. Atoms not involved are omitted.

Table 5. *Interatomic distances less than* 3·3 Å *and related angles*

i	x,	y,	z
ii	x,	$1+y$,	z
iii	$-x$,	$-y$,	$-z$
iv	$-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$

N–O(3^{i})	2·842* Å	O(3^{i})—N–O(3^{iii})	92·3°
N–O(3^{iii})	2·790*	O(3^{i})—N–O(3^{iv})	126·0
N–O(3^{iv})	3·027*	O(3^{i})—N–O(4^{ii})	123·8
N–O(4^{ii})	2·786*	O(3^{iii})–N–O(3^{iv})	114·5
N–O(4^{iv})	3·221	O(3^{iii})–N–O(4^{ii})	109·0
		O(3^{iv})–N–O(4^{ii})	91·2

* Hydrogen bonds.

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