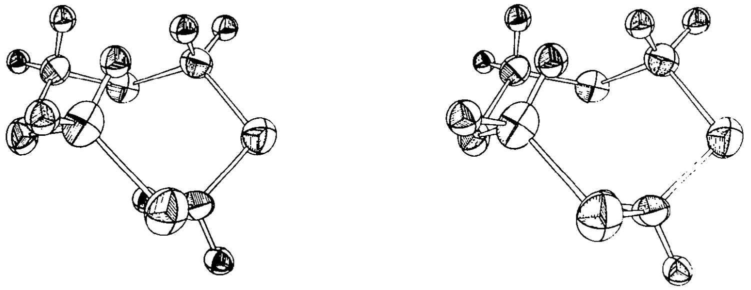

Fig. 6. Stereo *ORTEP* drawing of ring *A*, showing thermal ellipsoids, staggered view.

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The Crystal Structure of Acetophenone at 154 °K

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The crystal and molecular structure of acetophenone, $C_6H_5COCH_3$, has been determined by three-dimensional X-ray data collected by diffractometry at 154 °K. The crystals are monoclinic, space group $P2_1/n$ with cell dimensions: $a = 10{\cdot}256$ (1), $b = 8{\cdot}678$ (2), $c = 8{\cdot}558$ (1) Å, $\beta = 121{\cdot}00$ (1)° and $Z = 4$. The structure was solved by the symbolic addition procedure and refined by the block-diagonal least-squares method to give $R = 0{\cdot}038$ for the 1237 observed reflexions. The molecule is nearly planar. The methyl carbon atom deviates from the plane of the benzene ring by 0·121 Å. The C=O bond length is 1·216 (2) Å. The molecules are packed by van der Waals forces.

Introduction

Analysis of the Zeeman splitting pattern of the acetophenone crystal requires a knowledge of the crystal structure (Tanimoto, Kobayashi, Nagakura & Azumi, 1972). Acetophenone was subjected to X-ray crystal analysis at 154 °K in order to obtain accurate structural parameters.

Experimental

Crystals were obtained by standing an ethanol solution in a refrigerator. A small spherical crystal of about 0·5 mm in diameter was used. The cooling device is broadly similar to that described by Post, Schwartz & Fankuchen (1951). The crystal specimen was cooled by a flow of cold nitrogen gas surrounded by a jacket of dry nitrogen gas at room temperature, both issuing from an evaporation vessel containing liquid nitrogen. The liquid level in the evaporation vessel was auto-

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matically kept constant by supplying liquid nitrogen from a larger reservoir. Measurement by thermocouple indicated that the temperature of the crystal was 154 ± 2 °K throughout the experiment.

Intensity data were collected using a Rigaku automated four-circle diffractometer equipped with the cooling device, and Mo $K\alpha$ radiation monochromated by a graphite crystal. The ω-scan technique was employed. Data were recorded for 1555 independent reflexions up to $2\theta=55°$, of which 1237 with $|F|>3\sigma$ were regarded as 'observed'. Three standard reflexions were measured every fifty reflexions. The intensities were corrected for Lorentz and polarization effects, but corrections for absorption and extinction were not applied.

Crystal data are: C_8H_8O, M.W. 120·2, m.p. 20 °C. Monoclinic, $a=10{\cdot}256$ (1), $b=8{\cdot}678$ (2), $c=8{\cdot}558$ (1) Å, $\beta=121{\cdot}00$ (1)°. at 154°K, $U=652{\cdot}9$ Å^3, $Z=4$, $D_x=1{\cdot}222$ g cm^{-3}. Space group $P2_1/n$ (No. 14). Linear absorption coefficient for Mo $K\alpha$, $\mu=0{\cdot}79$ cm^{-1}.

Structure determination

The structure was solved by obtaining phases with the aid of the symbolic addition procedure for centrosymmetric crystals. The $\sum_2$ relationships for reflexions with $|E|\geq 1{\cdot}6$ were listed and the associated probabilities were calculated. Phases were determined for 73 reflexions with probabilities larger than 0·98. On the resulting E map the nine prominent peaks defined all the non-hydrogen atoms. The coordinates of the non-hydrogen atoms were refined by the block-diagonal least-squares method with unit weight being given to all the observed reflexions. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1962). After several cycles the refinement converged at $R=0{\cdot}13$. A difference Fourier synthesis at this stage revealed the positions of eight hydrogen atoms. Further refinement was carried out in anisotropic modes, but the thermal parameters of the hydrogen atoms were assumed to be isotropic. The R index dropped to 0·037 for the 1237 observed reflexions. At the final stage of the refinement, all the parameter shifts were less than one tenth of their standard deviations. The final atomic positional and thermal parameters, together with their estimated standard deviations, are listed in Table 1. The calculated structure amplitudes are compared with the observed values in Table 2.

Table 1. *Atomic parameters*

Positional and thermal parameters for the non-hydrogen atoms (× 10^4), with their e.s.d.'s in parentheses. The B_{ij}'s are defined by: $\exp[-(h^2B_{11}+k^2B_{22}+l^2B_{33}+hkB_{12}+hlB_{13}+klB_{23})]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
C(1)	3745 (2)	8185 (2)	4194 (2)	66 (2)	70 (2)	85 (2)	−19 (3)	79 (3)	−17 (3)
C(2)	4004 (2)	7103 (2)	5524 (2)	117 (2)	70 (2)	127 (3)	3 (3)	145 (4)	9 (4)
C(3)	3286 (2)	7250 (2)	6514 (2)	152 (3)	89 (2)	138 (3)	−35 (4)	196 (5)	14 (4)
C(4)	2313 (2)	8470 (2)	6194 (2)	101 (2)	120 (2)	126 (3)	−46 (4)	157 (4)	−42 (4)
C(5)	2056 (2)	9555 (2)	4882 (2)	93 (2)	127 (2)	128 (3)	43 (4)	136 (4)	10 (4)
C(6)	2768 (2)	9411 (2)	3876 (2)	84 (2)	95 (2)	103 (2)	28 (3)	108 (4)	28 (4)
C(7)	4524 (2)	7975 (2)	3138 (2)	69 (2)	78 (2)	97 (2)	−20 (3)	86 (3)	−28 (3)
C(8)	4168 (2)	9066 (2)	1611 (2)	96 (2)	112 (2)	111 (3)	−6 (3)	134 (4)	14 (4)
O	5409 (1)	6912 (1)	3500 (2)	114 (2)	107 (2)	174 (2)	54 (3)	187 (3)	10 (3)

Table 1 (*cont.*)

Positional (× 10^3) and isotropic thermal parameters for the hydrogen atoms.

	x	y	z	B
H(1)	469 (2)	623 (2)	572 (2)	1·8 (3)
H(2)	351 (2)	645 (2)	748 (3)	3·1 (5)
H(3)	180 (2)	864 (2)	693 (3)	2·2 (4)
H(4)	136 (2)	1044 (2)	467 (3)	2·3 (4)
H(5)	260 (2)	1025 (2)	296 (3)	2·1 (4)
H(6)	438 (2)	1014 (2)	202 (3)	2·4 (4)
H(7)	479 (2)	881 (2)	106 (3)	2·2 (4)
H(8)	305 (2)	896 (2)	63 (3)	2·0 (4)

Description of the structure and discussion

A projection of the structure along the b axis is presented in Fig. 1. Bond lengths and angles are shown in Fig. 2. The molecule is essentially planar. Table 3 lists the displacements of the atoms from the best plane of the benzene ring. The methyl carbon atom deviates from the plane of the benzene ring by 0·121 Å, whereas the oxygen atom is displaced by −0·027 Å. The C(1)–C(7) bond is inclined at 0·73° to the plane of the benzene ring. The dihedral angles C(2)C(1)C(7)C(8) and C(6)C(1)C(7)O are 4·40 and 2·35° respectively. All the bond lengths and angles are normal. The C=O bond length of 1·216 Å may be compared with the corresponding values observed in many organic crystals (for example, Birnbaum, 1973; Dideberg, Campsteyn & Dupont, 1973). Table 4 lists interatomic distances between molecules which are packed by van der Waals forces. The closest contact of 3·379 Å occurs between C(5) and O. In Fig. 1 are superposed sections of the residual electron density map through the bond centres and the centre of the benzene ring. The systematic arrangement of the maxima and minima seems to suggest that the electron density has moved to the centre of the bonds. In the middle of the C=O bond no maxima appears, probably for the same reason that applies to *cis*-1,2,3-tricyanocyclopropane (Hartman & Hirshfeld, 1966) and a 1,2,4,5-tetracyanobenzene complex (Tsuchiya, Marumo & Saito, 1972).

Table 2. *Observed and calculated structure factors*

H	K	L	10FO	10FC
0	0	2	88	89
0	0	4	344	-338
0	0	6	187	187
0	1	1	277	-283
0	1	3	151	-146
0	1	4	76	76
0	1	5	43	41
0	1	6	16	-17
0	1	7	50	49
0	1	8	77	-77
0	2	0	437	-440
0	2	1	224	223
0	2	2	127	129
0	2	3	131	123
0	2	4	172	164
0	2	5	69	65
0	2	6	14	-13
0	2	7	45	47
0	2	8	73	73
0	2	9	30	-30
0	3	1	166	-168
0	3	2	84	63
0	3	3	37	-31
0	3	4	144	-137
0	3	5	52	-49
0	3	6	8	7
0	3	7	80	-84
0	3	8	14	15
0	4	0	58	56
0	4	1	77	77
0	4	2	33	33
0	4	3	40	41
0	4	4	61	61
0	4	5	146	-149
0	4	6	36	38
0	4	7	47	-50
0	4	8	20	-19
0	5	1	27	28
0	5	2	19	-19
0	5	3	11	4
0	5	4	31	-31
0	5	5	36	-36
0	5	6	38	43
0	5	7	37	41
0	5	8	19	20
0	6	0	51	47
0	6	1	96	97
0	6	3	100	103
0	6	5	44	43
0	6	6	48	-49
0	6	7	15	15
0	6	8	6	-9
0	7	1	63	-64
0	7	2	172	-172
0	7	3	35	37
0	7	4	22	22
0	7	5	24	24
0	7	6	25	-24
0	8	0	172	-175
0	8	1	101	-105
0	8	2	26	-27
0	8	3	33	-31
0	8	4	40	38
0	8	5	49	46
0	9	1	120	122
0	9	2	69	70
0	9	3	6	-13
0	9	4	26	-24
0	9	5	47	-42
0	10	0	53	52
0	10	1	17	15
0	10	2	24	-26
0	10	3	8	-7
1	0	-9	81	-83
1	0	-7	49	-47
1	0	-5	48	46
1	0	-3	165	-170
1	0	-1	[illegible]	[illegible]
1	0	1	384	388
1	0	3	208	-202
1	0	5	89	-83
1	0	7	34	-36
1	0	9	8	6
1	1	-9	43	-45
1	1	-8	40	38
1	1	-7	20	22
1	1	-6	16	-13
1	1	-5	88	-18
1	1	-4	37	-36
1	1	-3	129	123
1	1	-1	84	-82
1	1	0	73	-75
1	1	1	783	-820
1	1	2	208	202
1	1	3	51	47
1	1	4	121	117
1	1	5	186	182
1	1	6	10	10
1	1	7	21	23
1	2	-9	111	113
1	2	-8	101	99
1	2	-6	66	-64
1	2	-5	130	-132
1	2	-4	307	-297
1	2	-3	394	390
1	2	-2	109	107
1	2	-1	143	-150
1	2	0	527	532
1	2	1	698	-709
1	2	2	36	34
1	2	3	45	43
1	2	4	31	-26
1	2	6	44	47
1	2	7	10	-9
1	2	8	13	-12
1	3	-9	50	-51
1	3	-8	27	-28
1	3	-7	12	-12
1	3	-6	25	26
1	3	-5	36	35
1	3	-4	93	[illegible]
1	3	-3	21	[illegible]
1	3	-2	30	29
1	3	-1	8	10
1	3	0	101	-98
1	3	1	40	-38
1	3	2	15	14
1	3	3	134	-128
1	3	4	46	47
1	3	5	32	33
1	3	6	68	-69
1	3	7	23	-23
1	3	8	31	-32
1	4	-9	36	-39
1	4	-8	34	33
1	4	-7	11	-17
1	4	-6	175	135
1	4	-5	44	40
1	4	-4	81	77
1	4	-3	135	-128
1	4	-2	201	190
1	4	-1	101	98
1	4	0	113	111
1	4	1	123	118
1	4	3	79	-81
1	4	5	6	-1
1	4	6	27	-27
1	4	7	41	44
1	4	8	28	32
1	5	-7	40	-46
1	5	-6	30	32
1	5	-5	46	-43
1	5	-4	74	-77
1	5	-3	87	-83
1	5	-2	154	-152
1	5	-1	130	-134
1	5	0	141	144
1	5	1	22	-20
1	5	2	159	161
1	5	3	12	16
1	5	4	56	-60
1	5	5	28	-28
1	5	6	67	70
1	5	7	29	-31
1	5	8	40	42
1	6	-8	15	15
1	6	-7	21	21
1	6	-6	50	-52
1	6	-5	44	48
1	6	-4	12	10
1	6	-3	90	-91
1	6	-2	38	-36
1	6	-1	37	38
1	6	0	32	29
1	6	1	106	112
1	6	2	100	100
1	6	3	39	-37
1	6	4	33	32
1	6	5	36	-36
1	6	6	38	42
[illegible]	[illegible]	[illegible]	[illegible]	-18
1	[illegible]	[illegible]	[illegible]	-16
1	7	-4	19	-20
1	7	-3	15	14
1	7	-2	93	88
1	7	-1	30	-33
1	7	0	21	-22
1	7	1	158	-167
1	7	2	170	-184
1	7	3	48	-48
1	7	4	23	-20
1	7	5	27	28
1	7	6	[illegible]	[illegible]
1	7	7	[illegible]	[illegible]
1	8	-7	36	[illegible]
1	8	-6	25	26
1	8	-5	9	11
1	8	-4	13	-13
1	8	-2	83	81
1	8	-1	128	-127
1	8	0	[illegible]	[illegible]
1	8	1	78	-28
1	8	2	45	41
1	8	3	101	100
1	8	4	24	-28
1	8	6	36	-38
1	9	-6	48	-38
1	9	-5	38	36
1	9	-4	19	19
1	9	-2	31	31
1	9	-1	70	-70
1	9	0	16	[illegible]
1	9	1	68	[illegible]
1	9	2	32	37
1	9	3	14	15
1	9	4	26	-29
1	9	5	51	-42
1	10	-4	71	68
1	10	-3	24	-24
1	10	-2	27	-28
1	10	-1	58	55
1	10	0	68	-79
1	10	1	33	35
1	10	2	25	29
1	11	-1	21	26
1	11	0	37	-30
1	11	1	17	-14
2	0	-10	59	-61
2	0	-8	281	-283
2	0	-6	72	73
2	0	-4	88	87
2	0	-2	520	-534
2	0	0	69	-67
2	0	2	64	-62
2	0	4	45	-40
2	0	6	69	57
2	1	-10	15	17
2	1	-9	56	50
2	1	-8	115	115
2	1	-7	27	26
2	1	-6	10	-33
2	1	-5	40	39
2	1	-4	186	-187
2	1	-3	241	-239
2	1	-2	270	285
2	1	-1	114	-113
2	1	0	514	-532
2	1	1	647	650
2	1	2	310	-301
2	1	3	14	14
2	1	4	173	164
2	1	5	74	-71
2	1	6	50	49
2	1	7	40	47
2	1	8	38	39
2	2	[illegible]	45	46
2	2	[illegible]	47	41
2	2	[illegible]	68	-69
2	2	[illegible]	91	-90
2	2	[illegible]	70	-71
2	2	-4	10	-9
2	2	[illegible]	113	-117
2	2	[illegible]	366	-361
2	2	[illegible]	107	-100
2	2	[illegible]	27	-25
2	2	[illegible]	[illegible]	-13
2	2	[illegible]	45	-42
2	2	[illegible]	26	-27
2	2	[illegible]	25	-22
2	3	[illegible]	67	-68
2	3	[illegible]	43	37
2	3	[illegible]	122	111
2	3	-6	176	176
2	3	[illegible]	326	317
2	3	[illegible]	191	-186
2	3	[illegible]	241	242
2	3	[illegible]	106	103
2	3	[illegible]	306	-293
2	3	[illegible]	293	289
2	3	[illegible]	54	-51
2	3	[illegible]	25	-23
2	3	[illegible]	57	57
2	3	[illegible]	36	-37
2	3	[illegible]	41	-42
2	4	[illegible]	12	-10
2	4	[illegible]	32	-27
2	4	[illegible]	41	-43
2	4	[illegible]	36	37
2	4	[illegible]	81	-75
2	4	[illegible]	168	160
2	4	[illegible]	92	-98
2	4	[illegible]	62	-63
2	4	[illegible]	103	-96
2	4	[illegible]	34	31
2	4	[illegible]	10	10
2	4	[illegible]	17	18
2	4	[illegible]	61	-61
2	4	[illegible]	21	-21
2	4	[illegible]	20	22
2	5	[illegible]	20	22
2	5	-7	13	-12
2	5	-6	14	20
2	5	-5	84	-88
2	5	-4	30	34
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2	5	-1	110	-103
2	5	0	49	-50
2	5	1	119	121
2	5	2	140	149
2	5	3	121	125
2	5	4	81	80
2	5	5	13	11
2	5	6	53	-54
2	5	7	16	21
2	6	-7	50	-58
2	6	-6	9	10
2	6	-5	87	-92
2	6	-4	10	-8
2	6	-3	10	-8
2	6	-2	94	87
2	6	-1	77	74
2	6	0	46	42
2	6	1	[illegible]	[illegible]
2	6	2	92	-94
2	6	3	149	-152
2	6	4	15	-13
2	6	5	17	21
2	6	6	24	22
2	7	-8	46	45
2	7	-7	39	37
2	7	-6	70	72
2	7	-4	73	-75
2	7	-3	21	16
2	7	-2	25	22
2	7	-1	78	80
2	7	0	7	8
2	7	1	102	-107
2	7	2	72	-76
2	7	3	76	-76
2	7	4	48	46
2	7	5	33	32
2	7	6	62	62
2	8	-7	35	34
2	8	-6	30	-28
2	8	-3	30	-38
2	8	-2	15	18
2	8	-1	59	60
2	8	0	32	-32
2	8	1	48	49
2	8	2	71	70
2	8	4	15	15
2	8	5	33	-33
2	9	-6	20	-27
2	9	-5	28	24
2	9	-4	27	27
2	9	-3	41	40
2	9	-2	12	13
2	9	-1	81	-83
2	9	0	75	74
2	9	1	29	-26
2	9	2	28	26
2	9	3	30	31
2	9	4	26	-25
2	10	-5	22	22
2	10	-4	48	-43
2	10	-2	32	-32
2	10	-1	60	-65
2	10	0	107	109
2	10	1	44	-43
2	10	2	24	23
2	11	-1	16	-18
2	11	0	32	-30
3	0	-9	42	-42
3	0	-7	65	66
3	0	-5	59	59
3	0	-3	89	-76
3	0	-1	182	187
3	0	1	70	-65
3	0	3	46	42
3	0	5	147	150
3	0	7	21	20
3	1	-9	96	96
3	1	-8	13	12
3	1	-7	[illegible]	281
3	1	-6	66	-68
3	1	-5	228	-225
3	1	-4	230	-217
3	1	-3	336	-326
3	1	-1	280	276
3	1	0	53	-53
3	1	1	171	-171
3	1	2	52	-54
3	1	3	81	-81
3	1	4	42	-39
3	1	5	45	45
3	1	6	23	-22
3	1	7	28	28
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10	2	[illegible]	30	38
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10	3	[illegible]	33	32
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9	0	-3	103	104
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9	6	0	32	34
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9	8	-3	24	-25
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10	5	[illegible]	18	19
10	5	[illegible]	39	-38
10	5	[illegible]	80	-78
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10	5	[illegible]	49	48
10	5	[illegible]	21	-19
10	5	[illegible]	12	-12
10	6	[illegible]	61	-80
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10	6	-4	64	70
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10	7	[illegible]	17	16
10	7	[illegible]	[illegible]	4
10	7	[illegible]	44	42
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11	0	-7	38	-40
11	0	[illegible]	110	119
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11	1	-6	46	-47
11	1	-5	42	45
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11	2	-3	18	-15
11	2	-2	85	81
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11	3	-5	59	-57
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11	3	-1	14	17
11	4	-8	[illegible]	81
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11	4	-4	38	34
11	4	-3	16	13
11	4	-2	39	40
11	4	-1	19	19
11	5	[illegible]	[illegible]	[illegible]
11	5	[illegible]	42	-40
11	5	[illegible]	19	-18
11	5	[illegible]	40	-39
11	5	[illegible]	19	-18
11	6	[illegible]	37	36
11	6	[illegible]	13	-12

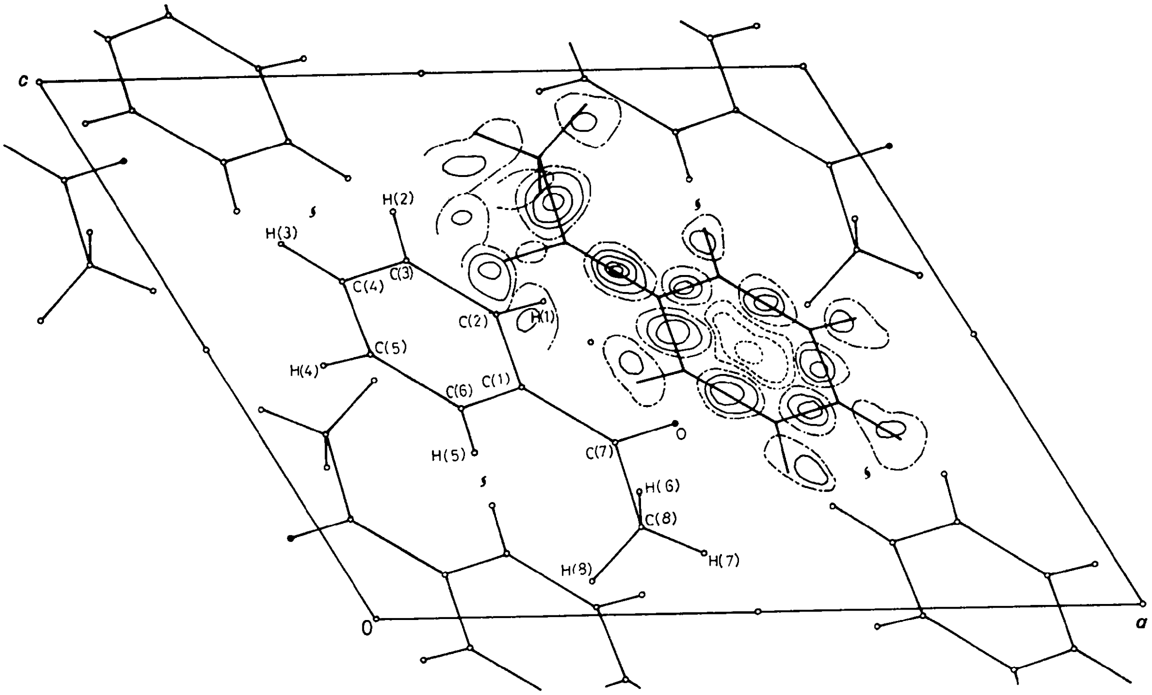

Fig. 1. A projection of the structure along the *b* axis. Sections of the residual electron density map through the bond centres and the centre of the benzene ring are superposed. The contours are at intervals of 0·05 e Å^{-3}. Negative contours are broken, zero being chained.

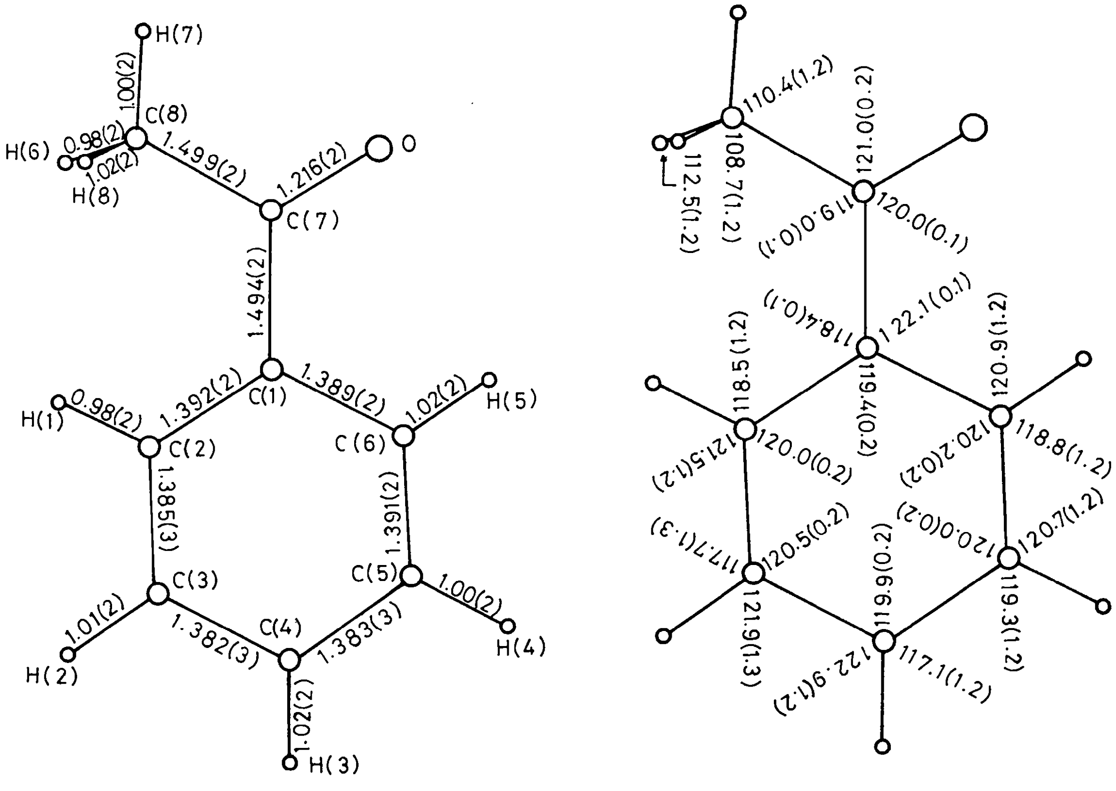

Fig. 2. Bond lengths (Å) and angles (°), with their standard deviations in parentheses.

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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$NH_4(CH_3)_2PO_4$ 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