The four C–O bonds in the two heterocyclic rings are within 2σ of the average value of 1·380 Å. The small differences are consistent with predictions based upon ring strain and electron delocalization. The C(8)–O(14) distance of 1·375 Å is similar to that found for many methoxyl groups attached to aromatic ring systems; however, the methoxyl group does not lie within the plane of the ring.

A unit weighted least-squares plane fitted to the six atoms comprising the benzene ring gives the equation $0{\cdot}2515x+0{\cdot}6273y-0{\cdot}7370z=1{\cdot}4022$. The average deviation of the six ring atoms from the plane is 0·005 Å with a maximum deviation of 0·009 Å. The five-membered ring is slightly puckered with O(12) 0·006 Å above the plane of the benzene ring and O(11) and C(13) below. The atoms of the six-membered heterocyclic ring lie above the plane and there is a slight folding of the ring about the O(1)–C(4) axis. If a least-squares plane is fitted to the atoms comprising the three rings the equation $0{\cdot}2517y+0{\cdot}6221y-0{\cdot}7414z=1{\cdot}3922$ is obtained. The maximum deviation from this plane is 0·02 Å indicating a reasonably planar system.

The methoxyl oxygen is 0·07 Å below the plane of the benzene ring while the methyl carbon is rotated to a position 0·94 Å above. The dihedral angle formed by the O(14)–C(15) bond with respect to the plane is 54·6°. If the methyl carbon lay in the plane of the ring, the electron pair of the oxygen would have the greatest overlap with the π orbitals of the aromatic ring system. This geometry is observed for most methoxyl groups attached to aromatic systems where there are no large substituents in the adjacent *ortho* positions, (Yonemitsu, Nakai, Kanaoka, Karle & Witkop, 1968; Corbin, Karle & Karle,1970; Gilardi & Karle, 1971; Ting, Watson & Dominguez, 1972). If the methyl carbon in xanthotoxin lay within the plane the C(15)–O(11) or the C(15)–O(1) distance would be 2·60 Å or 2·16 Å. The methyl group is sterically forced out of the plane and the angle of 54·6° is probably a compromise between steric repulsion and overlap of the oxygen electrons with the ring.

All intermolecular contact distances are greater than the sum of the van der Waals radii except for the O(16)–H(12) interaction distance of 2·26 Å. The C(12)–H(12)–O(16) angle is 141°. The easy cleavages along (100) and (010) are explained by molecular packing considerations. The perpendicular distance between molecular planes stacked along **c** is 3·58 Å, and the two molecules related by the **a** glide make an angle of 83°.

We would like to acknowledge The Robert A. Welch Foundation for their financial support and the TCU Research Foundation for the purchase of equipment.

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The Crystal and Molecular Structure of α-*p*-Dimethylaminobenzaldoxime

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(*Received* 14 *April* 1972)

Crystals of α-*p*-dimethylaminobenzaldoxime, $(CH_3)_2N.C_6H_4.CHNOH$, are monoclinic, $a=7{\cdot}705$, $b=6{\cdot}190$, $c=19{\cdot}149$ Å, $\beta=95{\cdot}80°$, space group $P2_1/c$, with four formula units in the unit cell. The structure was solved by Patterson and Fourier methods and refined by the full-matrix least-squares method, using 980 non-zero reflexions collected by the counter method, to a final R value of 0·059. Two centrosymmetrically related molecules interact through two O–H···N hydrogen bonds (2·784 Å), and the crystal is built up of discrete centrosymmetric quasi-planar dimers. The molecular structure is discussed on the basis of the observed bond lengths and angles.

The structure analysis of α-*p*-dimethylaminobenzaldoxime, $(CH_3)_2N.C_6H_4.CHNOH$, is part of a program involving a systematic study of the structure of *para*-substituted benzaldoximes and their methyl derivatives.

Experimental

Crystal data

α-*p*-Dimethylaminobenzaldoxime, $(CH_3)_2N.C_6H_4.CHNOH$ was prepared as described in the literature (Brady, Cosson & Roper, 1925). Colourless crystals suitable for single-crystal X-ray analysis were grown from benzene solutions, m.p. 144°C. The crystals are stable in air and to X-rays. Preliminary X-ray and optical examinations of the crystals indicated that they are monoclinic. The space group, $P2_1/c$ (No. 14), was assigned on the basis of the systematic absences ($h0l$, $l=2n+1$; $0k0$, $k=2n+1$).

The unit-cell dimensions at ~23°C are: $a=7{\cdot}705\pm0{\cdot}003$, $b=6{\cdot}190\pm0{\cdot}003$, $c=19{\cdot}149\pm0{\cdot}005$ Å, $\beta=95{\cdot}80\pm0{\cdot}03°$; they were determined by a least-squares fit of the setting angles of sixteen strong reflexions centred on a Siemens AED automatic diffractometer using Mo $K\alpha$ radiation ($\lambda=0{\cdot}7107$ Å). The density, $1{\cdot}20\pm0{\cdot}01$ g.cm^{-3}, measured by flotation in $Ca(NO_3)_2$ solution agrees well with the value 1·200 g.cm^{-3} calculated for four formula units of molecular weight 164·208 in the cell volume of 908·56 Å^3.

Intensity data were collected in the ω-scan mode with Mo $K\alpha$ radiation filtered through a 0·05 mm Zr foil. A fixed symmetrical scan range of 0·65° from the computed Mo $K\alpha$ peak was used. Each reflexion was scanned twice, and stationary-crystal stationary-counter background counts were taken for a time equal to the scan time at each end of the scan. 1450 independent reflexions were recorded for θ(Mo $K\alpha$) $\le 24°$: at higher values of θ very few reflexions had intensities above the background. Four standard reflexions, chosen in different regions of reciprocal space, were measured every 80 reflexions and their intensities remained effectively constant throughout the run. The data were processed as previously described (Cerrini, Colapietro, Spagna & Zambonelli, 1971). The crystal used measured 0·1 × 0·3 × 0·6 mm and was mounted with the long dimension coincident with the polar ϕ axis. No absorption correction was necessary since μ(Mo $K\alpha$) = 1·14 cm^{-1} and no extinction correction was applied. Of the 1450 collected reflexions, 230 were discarded, mainly because their peak intensities were less than or equal to the background counts. Altogether 240 reflexions with $F_0^2 \le \sigma(F_0^2)$ were classified as unobserved and excluded from the last cycles of refinement.

Structure determination

A three-dimensional temperature-sharpened Patterson map was calculated using all the 1220 reflexions: the F_0^2 values were multiplied by exp $(4\sin^2\theta/\lambda^2)$.

The relative coordinates of the carbon atoms of the benzene ring and of the two atoms directly bound to it (without any distinction between the two atoms) were obtained from well defined peaks near the origin. These eight atoms were then shifted from the region near the origin by a displacement vector which could be determined both from the Harker peaks on the section at $P(u,\frac{1}{2},w)$ and the composite vector peaks originating from the set of vectors between centrosymmetrically related molecules. From a three-dimensional Fourier synthesis phased on the contribution of these eight atoms it was possible to locate all the non-hydrogen atoms.

An isotropic full-matrix least-squares refinement of all the non-hydrogen atoms, using all the reflexions with unit weights, reduced R from 0·30 to 0·188. Refinement was continued allowing the atoms to vibrate anisotropically: convergence was reached at $R=0{\cdot}128$. A difference Fourier synthesis calculated at this stage showed the positions of all the hydrogen atoms. The introduction of the hydrogen atoms in the structure

Table 1. *Final positional and thermal parameters with their estimated standard deviations*

Fractional coordinates are given. The general form of the anisotropic temperature factors is:

$$\exp\{-[h^2B(11)+k^2B(22)+l^2B(33)+hkB(12)+hlB(13)+klB(23)]\times10^{-4}\}.$$

Parameters for carbon, nitrogen and oxygen atoms are $\times 10^4$; positional parameters for the hydrogen atoms are $\times 10^3$.

	X	Y	Z	B(ISO)	B(11)	B(12)	B(13)	B(22)	B(23)	B(33)
C(1)	1268(4)	2215(5)	1711(1)		237(7)	76(14)	30(4)	321(10)	−2(5)	35(1)
C(2)	1351(4)	629(6)	2221(2)		227(7)	−47(15)	27(5)	319(11)	7(6)	44(1)
C(3)	2272(4)	899(5)	2868(2)		270(8)	−41(15)	16(5)	284(10)	39(6)	41(1)
C(4)	3188(4)	2788(5)	3041(1)		212(6)	−1(13)	23(4)	289(10)	13(5)	38(1)
C(5)	3147(4)	4391(5)	2524(2)		249(7)	−62(15)	31(5)	293(11)	18(6)	40(1)
C(6)	2223(4)	4102(6)	1878(2)		283(8)	21(15)	41(5)	311(11)	30(6)	38(1)
C(7)	266(5)	1865(7)	1031(2)		297(9)	102(19)	14(5)	399(14)	−33(7)	41(1)
C(8)	4029(11)	1481(9)	4236(3)		562(19)	−187(29)	−62(9)	429(17)	77(9)	46(2)
C(9)	4856(8)	5096(9)	3907(3)		359(12)	−327(26)	−28(7)	498(17)	18(9)	50(2)
N(1)	128(4)	3314(5)	563(1)		354(8)	142(15)	−9(4)	447(12)	−21(6)	36(1)
N(2)	4133(4)	3054(4)	3686(1)		344(7)	−120(14)	−27(4)	352(10)	25(5)	42(1)
O	−951(4)	2653(5)	−44(1)		493(8)	85(16)	−77(4)	556(11)	−48(5)	41(1)
H(1)	73(4)	−74(5)	212(1)	3,1(7)						
H(2)	234(4)	−33(5)	316(1)	3,1(7)						
H(3)	384(4)	572(5)	261(2)	3,7(7)						
H(4)	231(4)	522(5)	153(2)	3,4(7)						
H(5)	−28(4)	47(6)	93(2)	5,0(9)						
H(6)	−30(6)	426(9)	−42(2)	10,3(14)						
H(7)	428(5)	7(7)	406(2)	7,3(13)						
H(8)	280(8)	139(10)	441(3)	12,9(24)						
H(9)	501(7)	177(8)	456(3)	9,8(16)						
H(10)	578(6)	490(7)	430(2)	7,4(12)						
H(11)	401(8)	597(10)	402(3)	14,1(28)						
H(12)	542(6)	579(8)	349(2)	9,7(14)						

factor calculation, with the isotropic temperature factors previously obtained for the atoms to which they are bonded, decreased the R value to 0·109.

From this stage the refinement was continued with anisotropic temperature factors for the heavy atoms and isotropic temperature factors for the hydrogen atoms, using only the 980 observed reflexions; weights $w=[a+|F_o|+b|F_o|^2]^{-1}$, where $a=10{\cdot}00$ and $b=-0{\cdot}07$, were adjusted to keep constant the average $\langle w|\Delta F|^2\rangle$ for groups of F_o (Cruickshank, 1965). Convergence was reached at $R=0{\cdot}059$ for the 930 observed reflexions and $R=0{\cdot}072$ for all the reflexions.

Table 1 gives the final positional and thermal parameters of the atoms. The final values of observed and calculated structure factors (in electrons ×10) are listed in Table 2.

Atomic form factors given by Cromer & Mann (1968) for oxygen, nitrogen and carbon, and by Hanson, Herman, Lea & Skillman (1964) for hydrogen were used. Calculations were carried out on the UNIVAC 1108 computer of Rome University and were performed with the system of programs developed in this Laboratory (Domenicano, Spagna & Vaciago, 1969), with the extensive contribution of J. R. Carruthers.

Table 2. *Observed and calculated structure factors* (*in electrons* ×10)

$F(000)=352.$

K	L	FO	FC
•••• H = 0 ••••			
0	4	55	50
0	6	135	-143
0	8	29	-26
0	10	214	214
0	12	36	25
0	-14	28	21
0	-16	100	101
0	18	41	40
0	20	24	24
1	1	34	-27
1	-2	39	41
1	3	184	-193
1	4	56	-60
1	5	265	-265
1	-6	10	7
1	-7	141	138
1	-8	37	40
1	-9	254	247
1	10	163	162
1	-11	64	-58
1	12	14	-20
1	13•	8	-3
1	-14	37	38
1	15	72	-73
1	-16	142	-146
1	17	29	19
1	-18	14	-16
1	19	12	6
1	20	24	-17
2	0	228	-232
2	1	44	-43
2	2	407	-407
2	3	82	-83
2	4	83	89
2	5	76	-77
2	-6	345	-340
2	7	124	126
2	-8	54	49
2	9	97	96
2	10	54	-52
2	-11	55	58
2	12	41	-45
2	13	30	-32
2	14	48	-50
2	15	128	-126
2	16	64	-62
2	-17	66	-67
2	18	18	-16
2	19	30	-33
2	20•	14	-9
3	1	110	114
3	2	61	-60
3	-3	231	222
3	4	99	103
3	-5•	9	-9
3	-6	48	41
3	7	170	-164
3	9	45	-38
3	10	52	-48
3	11	25	-26
3	12	37	-37
3	13	49	50
3	-14	56	-57
3	-15	19	16
3	16	28	-27
3	-17	20	20
3	-18	22	23
3	-19	16	13
4	0	70	67
4	-1	40	39
4	-2	24	20
4	4	27	-11
4	6	94	101
4	-7•	9	2
4	8	78	77
4	-9	14	14
4	-10	34	38
4	-11	45	50
4	12	37	31
4	-13	126	-127
4	-14	18	-13
4	-15	34	34
4	-16	16	10
4	17	17	21
4	-18	23	12
5	1	66	74
5	2	26	-24
5	3	161	-160
5	4	21	19
5	-5	24	17
5	6	16	11
5	-7	18	-13
5	-8	17	-13
5	-9	33	31
5	10	22	20
5	11	35	36
5	-13	49	-48
5	-14	27	20
5	-15•	9	1
6	0	50	-49
6	1•	11	18
6	-2	95	96
6	-3	15	11
6	-4	83	-80
6	5	15	10
6	6	34	-35
6	-7•	11	15
6	-8•	11	10
6	-10	27	-24
7	1	16	-19
7	3	18	23
•••• H = 1 ••••			
0	2	328	317
0	-2	132	121
0	4	590	589
0	-4	332	336
0	6	218	212
0	8	300	-289
0	-8	37	42
0	10	150	146
0	-10•	3	-16
0	12	17	16
0	-12	115	112
0	14	40	-37
0	-14	76	78
0	16	45	49
0	-16	92	-88
0	18	77	79
0	-18	122	121
0	20	19	17
0	-20•	13	21
1	0	663	-700
1	1	140	-137
1	2	169	-165
1	3•	7	-8
1	-3	41	35
1	4	21	21
1	-4	240	244
1	-5	145	143
1	6	31	32
1	-6	40	44
1	7	109	-106
1	-7	103	-99
1	8	259	259
1	-8	174	171
1	9	118	113
1	-9	73	-69
1	10	61	70
1	-10	85	-85
1	11•	9	-10
1	-11	92	92
1	12	99	104
1	-12	18	15
1	13	140	141
1	-13	15	-23
1	14	87	91
1	-14	32	-29
1	15	117	-114
1	-15	75	72
1	16•	12	18
1	-16	58	-53
1	17	27	32
1	-17	99	-96
1	18	24	21
1	-18	39	35
1	19	42	-43
1	-19	33	31
1	20	15	15
1	-20	19	10
1	-21	27	-24
2	0	291	-304
2	1	78	-77
2	-1	185	185
2	2	346	-350
2	-2	185	-182
2	3	136	137
2	-3	191	-190
2	4	59	57
2	-4	85	-83
2	5	212	207
2	-5	121	-117
2	6	49	-53
2	-6	67	59
2	7	29	-28
2	-7	282	-277
2	8	34	-36
2	-8	124	-124
2	9	110	-110
2	-9	55	54
2	10	92	-90
2	-10	35	-44
2	-11	145	141
2	12	107	-108
2	-12	119	-122
2	13	44	-54
2	-13	28	28
2	14	112	122
2	-14•	11	-10
2	15	15	13
2	-15	34	34
2	16	58	-57
2	-16	22	29
2	-17	23	-22
2	18	51	-54
2	-18	55	-55
2	-19•	8	2
2	-20	49	-43
2	-21•	9	-5
3	0	182	-190
3	1•	7	-14
3	2	215	206
3	-2	13	-10
3	3	69	72
3	-3	33	38
3	4	288	-283
3	-4	178	-180
3	5	173	168
3	-5	75	75
3	6	19	13
3	-6	135	130
3	7•	11	-7
3	-7	53	49
3	8	29	-29
3	-8	97	-93
3	9	55	-57
3	-9	35	-42
3	10	53	-53
3	-10•	9	-8
3	11	150	-149
3	-11	37	-37
3	12	16	-1
3	-12	24	-28
3	13	32	34
3	-13	29	-31
3	14	55	-56
3	-14•	6	-3
3	15	54	61
3	-15	62	60
3	16•	9	-16
3	17	13	-1
3	-17	17	14
3	18	20	-10
3	19	15	-4
3	-19•	8	-3
4	0•	2	-7
4	1	103	102
4	-1	28	26
4	2	35	37
4	-2	43	48
4	3	58	-56
4	-3	165	-168
4	4	18	19
4	-4	76	81
4	5	88	-86
4	-5	215	223
4	6	65	56
4	-6	29	31
4	7•	12	-10
4	-7	30	29
4	8	21	13
4	-8	11	5
4	9	22	16
4	-9	17	8
4	11	99	100
4	-11	23	-26
4	12	94	92
4	-12	38	43
4	-13	90	-89
4	-14	56	50
4	15	25	17
4	-15	27	27
4	17	17	0
4	-17	14	-9
5	0	66	-64
5	1	16	-15
5	2	145	144
5	-2	92	90
5	3	20	-16
5	-3	12	13
5	4	25	27
5	-4	129	-134
5	5	24	20
5	-5	27	28
5	7	22	-28
5	-7•	10	8
5	9	18	-21
5	-9	20	-24
5	-10	16	13
5	11	69	70
5	-11	16	-13
5	13	43	-41
5	-13	45	47
5	-15	55	-58
6	0	27	-22
6	1	85	-88
6	-1	20	20
6	2	19	24
6	-2	15	-12
6	3	44	43
6	-3	51	56
6	4•	8	1
6	5	31	-30
6	-5	47	-47
6	6	17	-23
6	-6•	11	-9
6	-7	14	13
6	8•	7	5
6	-8	30	-24
6	10	35	-33
6	11•	13	-11
6	-11•	5	-8
7	0•	7	9
7	1•	15	-9
7	2	36	-31
7	-2•	3	1
•••• H = 2 ••••			
0	0	222	228
0	2	100	102
0	4	256	-249
0	-4	636	-639
0	6	327	-317
0	-6	87	-94
0	8	214	211
0	-8	83	93
0	10	37	-36
0	-10	22	-18
0	12	15	-8
0	-12•	9	14
0	14	11	-5
0	-14	12	12
0	-16	15	-17
0	18	17	17
0	-18	111	107
0	20	15	10
0	-20	13	3
1	0	255	263
1	1	151	-148
1	-1	461	471
1	2	95	93
1	3	45	-45
1	-3	636	-675
1	4•	10	2
1	-4	212	207
1	5	36	-32
1	-5	84	84
1	6	59	-59
1	-6	159	166
1	7	121	123
1	-7	164	-164
1	8	270	270
1	-8	38	36
1	9	45	44
1	-9	225	224
1	10	87	87
1	-10	52	52
1	11	17	20
1	-11	82	85
1	12	19	18
1	-12	20	-17
1	13	45	-49
1	-13	74	-73
1	14	123	128
1	-14	48	54
1	15•	4	-4
1	-15	18	-13
1	16	92	102
1	-16	46	45
1	17•	13	11
1	-17	29	-27
1	18•	9	-1
1	-18	89	-87
1	19•	11	5
1	-19	18	12
1	-20	44	45
1	-21	15	-3
2	0	216	-217
2	1	145	-139
2	-1•	4	6
2	2	221	215
2	-2	220	-217
2	3	63	-65
2	-3	75	-85
2	4	171	-165
2	-4	47	-47
2	5	106	105
2	-5	48	-47
2	6	31	-23
2	-6	49	47
2	7	122	118
2	-7	13	17
2	8	57	56
2	-8	140	-131
2	9	33	32
2	-9	58	-64
2	-10	119	121
2	11	52	-52
2	-11	18	-19
2	12	21	20
2	-12	73	-71
2	13	172	-176
2	-13	60	64
2	14	47	-47
2	15	58	59
2	-15•	9	3
2	-16	31	-32
2	17	28	-32
2	-17	30	28
2	18	18	12
2	-18	14	-22
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2	-7•	11	1
2	-8•	13	-8

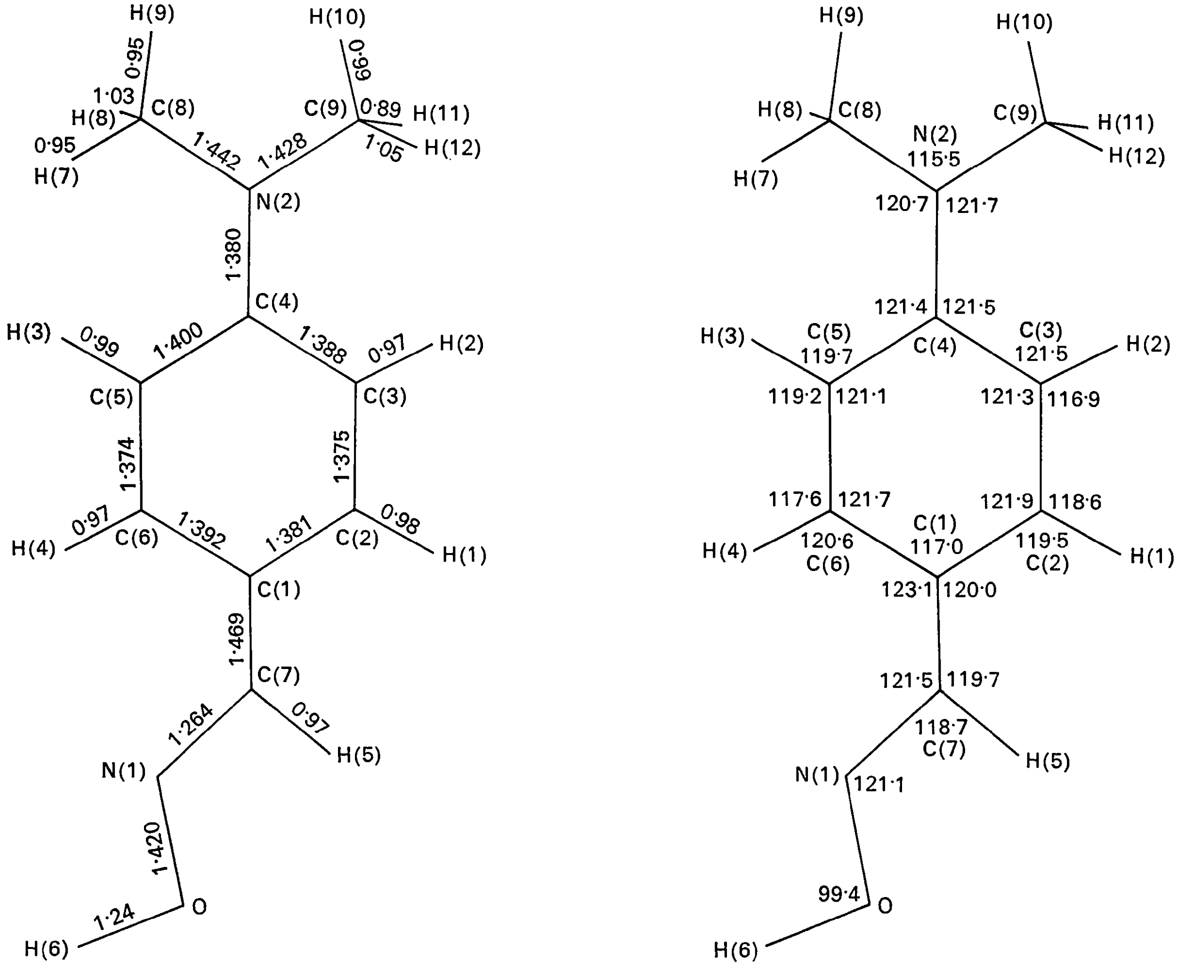

Fig. 1. Bond lengths and angles in the schematic projection of the molecule on the benzene plane.

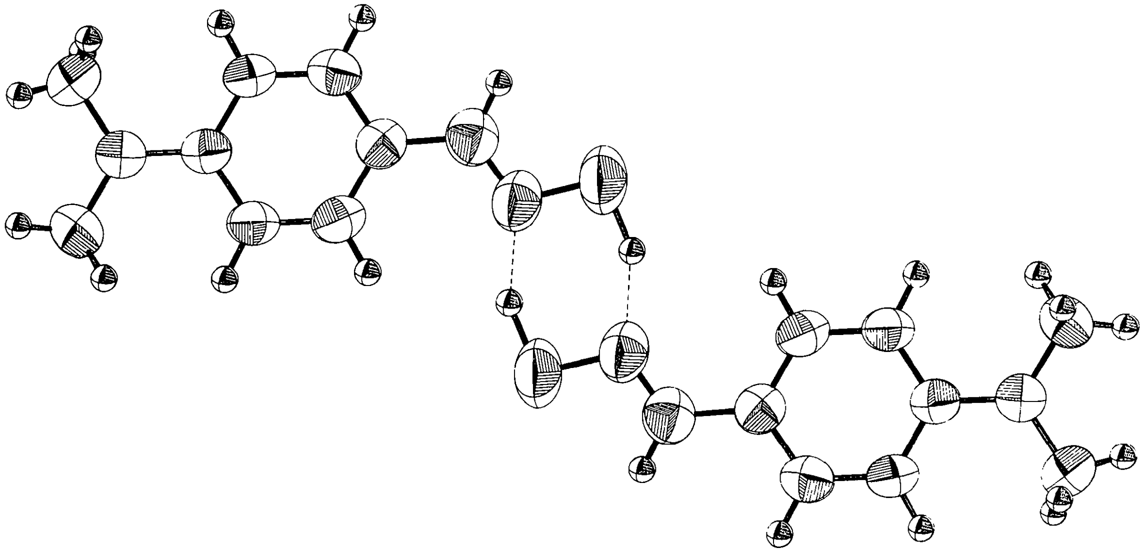

Fig. 2. Two centrosymmetrically related molecules linked by hydrogen bonds. The 50% probability contour of the thermal ellipsoids is shown for the non-hydrogen atoms. The figure was generated by Johnson's (1965) *ORTEP* program.

Results and discussion

An orthographic projection of the crystal-chemical unit on the plane of the benzene ring is given in Fig. 1. Intramolecular bond lengths and anglcs are given in Table 3.

Table 3. *Intramolecular bond lengths and angles with their estimated standard deviations*

The average values of the angles H–C–H and H–C–N(2) in the methyl groups are 109·37 and 109·47° respectively.

C(1)–C(2)	1·381 (5) Å	C(1)–C(2)–C(3)	121·9 (3)°
C(2)–C(3)	1·375 (5)	C(2)–C(3)–C(4)	121·3 (3)
C(3)–C(4)	1·388 (4)	C(3)–C(4)–C(5)	117·1 (3)
C(4)–C(5)	1·400 (4)	C(4)–C(5)–C(6)	121·1 (3)
C(5)–C(6)	1·374 (4)	C(5)–C(6)–C(1)	121·7 (3)
C(6)–C(1)	1·392 (5)	C(6)–C(1)–C(2)	117·0 (3)
C(1)–C(7)	1·469 (5)	C(2)–C(1)–C(7)	120·0 (3)
C(7)–N(1)	1·264 (5)	C(6)–C(1)–C(7)	123·1 (3)
N(1)–O	1·420 (4)	C(1)–C(7)–N(1)	121·5 (4)
C(4)–N(2)	1·380 (4)	C(7)–N(1)–O	112·1 (3)
N(2)–C(8)	1·442 (6)	C(3)–C(4)–N(2)	121·5 (3)
N(2)–C(9)	1·428 (6)	C(5)–C(4)–N(2)	121·4 (3)
C(2)–H(1)	0·98 (3)	C(4)–N(2)–C(8)	120·7 (3)
C(3)–H(2)	0·97 (3)	C(4)–N(2)–C(9)	121·7 (3)
C(5)–H(3)	0·99 (3)	C(8)–N(2)–C(9)	115·5 (4)
C(6)–H(4)	0·97 (3)	C(1)–C(2)–H(1)	119·5 (1·6)
C(7)–H(5)	0·97 (4)	C(3)–C(2)–H(1)	118·6 (1·6)
O——H(6)	1·24 (5)	C(2)–C(3)–H(2)	116·9 (1·7)
C(8)–H(7)	0·95 (5)	C(4)–C(3)–H(2)	121·5 (1·7)
C(8)–H(8)	1·03 (6)	C(4)–C(5)–H(3)	119·7 (1·7)
C(8)–H(9)	0·95 (5)	C(6)–C(5)–H(3)	119·2 (1·7)
C(9)–H(10)	0·99 (4)	C(5)–C(6)–H(4)	117·6 (1·7)
C(9)–H(11)	0·89 (7)	C(1)–C(6)–H(4)	120·6 (1·7)
C(9)–H(12)	1·05 (5)	C(1)–C(7)–H(5)	119·7 (2·0)
		N(1)–C(7)–H(5)	118·7 (2·0)
		N(1)–O——H(6)	99·4 (2·1)

In the solid state *α*-*p*-dimethylaminobenzaldoxime forms a centrosymmetrical dimer through two O–H···N hydrogen bonds (2·784 Å in length), as shown in Fig. 2.

The molecule is approximately planar. Relevant least-squares planes and deviations from them are given in Table 4.

I II

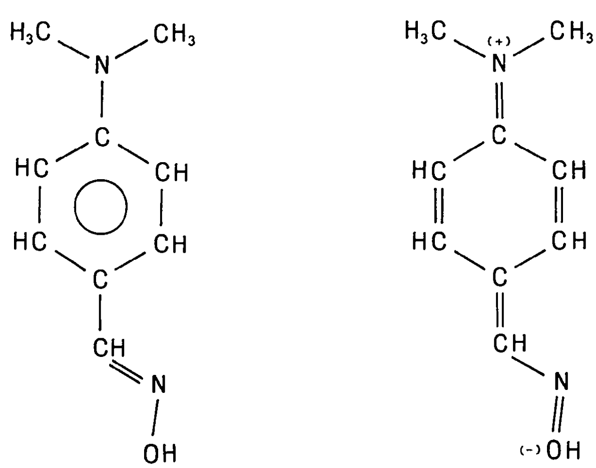

Fig. 3. Two possible cartonical forms of *α*-*p*-dimethylaminobenzaldoxime

Table 4. *Equations of least-squares planes and displacements of atoms from planes* (Å)

Planes are defined in terms of the crystallographic axes.

		Dihedral angles
$\varphi(1)$	$0{\cdot}857x - 0{\cdot}377y - 0{\cdot}436z = 1{\cdot}125$	$\varphi(2)\widehat{\ }\phi(3) = 2{\cdot}52^\circ$
$\varphi(2)$	$0{\cdot}849x - 0{\cdot}397y - 0{\cdot}433z = 1{\cdot}113$	$\varphi(2)\widehat{\ }\varphi(4) = 4{\cdot}63$
$\varphi(3)$	$0{\cdot}848x - 0{\cdot}368y - 0{\cdot}465z = 1{\cdot}178$	$\varphi(3)\widehat{\ }\varphi(4) = 5{\cdot}80$
$\varphi(4)$	$0{\cdot}888x - 0{\cdot}359y - 0{\cdot}377z = 0{\cdot}602$	

	$\varphi(1)$	$\varphi(2)$	$\varphi(3)$	$\varphi(4)$
C(1)	0·031	0·006	0·008	
C(2)	−0·017	−0·003		
C(3)	−0·023	−0·003		
C(4)	−0·043	0·005		0·032
C(5)	−0·073	−0·002		
C(6)	−0·069	−0·003		
C(7)	−0·005		0·010	
C(8)	0·094			0·029
C(9)	0·116			0·029
N(1)	0·034		−0·006	
N(2)	−0·067			−0·090
O	0·086		0·008	

Table 5. N–O *and* C=N *bond lengths in the oxime group of some alkyl and aryl oximes*

Compound	N–O	C=N	Reference
N-Methyl-*p*-chlorobenzaldoxime	1·284 (6)	1·309 (7)	Folting, Lipscomb & Jerslev (1964)
anti-2,6-Dimethyl-4-chloro-*N*-methylbenzaldoxime	1·298 (5)	1·299 (7)	Jensen & Jerslev (1969)
5-Chlorosalycilaldoxime	1·385 (13)	1·237 (16)	Simonsen, Pfluger & Thompson (1961)
anti-*p*-Chlorobenzaldoxime	1·39	1·26	Jerslev (1957)
syn-*p*-Chlorobenzaldoxime	1·408 (7)	1·260 (8)	Folting, Lipscomb & Jerslev (1964)
1,2-Benzodithiol-3-one oxime	1·418 (10)	1·309 (11)	Andreetti, Cavalca, Manfredotti & Musatti (1969)
α-*p*-Dimethylaminobenzaldoxime	1·420 (4)	1·264 (5)	Present work
Dimethylglyoxime*	1·321 (21)	1·253 (11)	Hamilton (1961)
Glyoxime	1·397 (5)	1·284 (5)	Calleri, Ferraris & Viterbo (1966)
Formaldoxime†	1·408	1·276	Levine (1963)
Formamidoxime	1·415 (28)	1·288 (35)	Hall (1965)

* Neutron diffraction study.

† Microwave study.

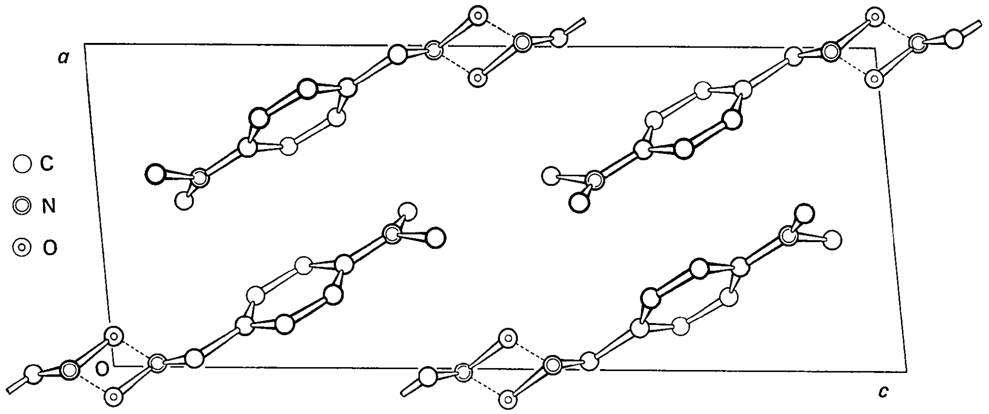

Fig. 4. Projection of the structure on the *ac* plane. Broken lines indicate O–H···N hydrogen bonds.

The six C–C bonds of the benzene ring, whose average length is 1·386 (2) Å, are not equivalent on the basis of statistical analysis and can be regarded as belonging to two different bond types: C(2)–C(3) and C(5)–C(6), whose average is 1·374 (3) Å, and the other four, whose average, 1·391 (2) Å, agrees well with the accepted value for the C–C bond in non-condensed aromatic molecules (Bastiansen & Skancke, 1961).

Accordingly, the angles in the ring, which average 119·7 (1)°, can also be regarded as belonging to two different types: the angles at C(1) and C(4) which average 117·0 (2)° and the other four which average 121·5 (2)°.

The C(4)–N(2) bond, 1·380 (4) Å, is distinctly shorter than a C(sp^2)–N single bond, 1·446 Å, as calculated from the sum of the single bond radii of C(sp^2) and N (Bastiansen & Skancke, 1961; Jönsson & Hamilton, 1970).

The C(1)–C(7) bond of 1·469 (5) Å agrees well with twice the C(sp^2) single bond radii, 1·474 Å (Bastiansen & Skancke, 1961).

The C(7)–N(1) bond, 1·264 (5) Å, is slightly longer than the accepted C–N double bond, 1·255 Å (Bayer & Häfelinger, 1966).

The N(1)–O bond, 1·420 (4) Å, is shorter (by 5σ) than the N–O single bond, 1·439 Å, calculated from the sum of O and N covalent radii (Pauling, 1960; and Jönsson & Hamilton, 1970).

In Table 5 the C=N and N–O bond lengths in the oxime group of some alkyl- and aryl-oximes are reported.

The geometry and the dimensions of the molecule of α-*p*-dimethylaminobenzaldoxime indicate that the canonical form II (Fig. 3) contributes, even though slightly, to the ground state of the molecule and that a diffuse delocalization involves the benzene ring, the nitrogen atom of the dimethylamino group and the oxime group. Such a conclusion is substantiated by the planarity of the dimethylamino group and the C(4)–N(2) bond length. Furthermore, although some bond lengths of the molecule differ insignificantly from the expected values for the canonical form I, all the bond lengths show a consistent trend towards the values expected for the canonical form II.

In Fig. 4 the packing mode of the molecules in the crystal is viewed in projection down the *b* axis.

Mr P. Mura gave technical assistance. We wish to thank Dr J. R. Carruthers for helpful discussions and for writing the least-squares program used in this work.

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