the thermal vibration is rather high, in accordance with the relatively low melting point. An analysis of the orientation of the ellipsoids indicates that their longest axes are nearly normal to plane (4) of the molecule, while the longest component in the molecular plane has a tendency to be parallel to a bond. This does not apply to the atoms bound to three other (non-hydrogen) atoms; these have a smaller thermal vibration and their ellipsoids are essentially revolution ones. The magnitude and anisotropy of the thermal parameters for atoms C(9) and O(2) are remarkable.

A short comparison of the characteristics of the two isomers is reported at the end of the following paper on the structure of the higher melting isomer.

The computations were done by Olivetti ELEA 6001 and IBM 7090 (C.N.U.C.E., Pisa) computers.

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The Crystal and Molecular Structure of the 5-Oxide of 4-Methyl-3-(*p*-Bromophenyl)-1,2,5-Oxadiazole

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The 5-oxide of 4-methyl-3-(*p*-bromophenyl)-1,2,5-oxadiazole, $BrC_6H_4–(C_2N_2O_2)–CH_3$, is the isomer of higher melting point (108–109 °C), obtained by oxidation of methyl(*p*-bromophenyl)glyoxime. It crystallizes in the monoclinic system, space group $P2_1/n$, with four molecules in a cell having: $a_0 = 12·648$, $b_0 = 10·136$, $c_0 = 7·499$ Å; $\beta = 94°52'$. A crystal-structure analysis has been based on all the X-ray reflexions accessible with Cu $K\alpha$ radiation. The molecule, approximately planar, has the configuration of furazan 5-oxide: the two isomers in question are positional isomers. The methyl group is involved in two intramolecular contacts with the extranuclear oxygen atom of the furoxan nucleus and with a hydrogen atom of the phenyl group. The molecular structures of the two isomers described in this and the preceding paper are compared.

As reported in the preceding paper (Calleri, Ferraris & Viterbo, 1969), which describes the structure of the lower melting point isomer of methyl(*p*-bromophenyl)furoxan, we are studying the isomerism of aryl-alkyl furoxans and, as a part of our programme the structure of the higher melting point isomer (HMI) of methyl(*p*-bromophenyl)furoxan is reported in the present paper.

Experimental

Crystal data and intensity measurement

In this case also, the compound prepared by Ponzio (1928*a,b*), was recrystallized from an aqueous-alcoholic solution, yielding prismatic crystals elongated in a direction chosen as the *c* axis. The following crystal data were obtained: $C_9H_7BrN_2O_2$; $M = 255·06$; m.p.

108–109 °C; Monoclinic prismatic; $a_0=12\cdot648\pm20\cdot0051$, $b_0=10\cdot1362\pm0\cdot0015$, $c_0=7\cdot4988\pm0\cdot0023$ Å, $\beta=94°\ 52'\pm2'$ (refined as for LMI); $V=957\cdot91$ Å^3; $D_m=1\cdot767$ g.cm^{-3} (by flotation); $Z=4$; $D_c=1\cdot768$ g.cm^{-3}; $F(000)=504$ e; Space group $P2_1/n$ (C_{2h}^5); Cu $K\alpha$ radiation; preliminary single-crystal rotation and Weissenberg photographs and subsequent single-crystal diffractometry; linear absorption coefficient $\mu=62\cdot67$ cm^{-1}.

The HMI crystal forms are the same as those of the lower melting isomer; again {110} is the predominant form and cleavage parallel to {$\bar{1}$01} is distinct.

The intensities were collected with a three-circle automatic diffractometer, using the same procedure described for the lower melting isomer; the crystal (about 0·6 mm long, cross section 0·10 × 0·12 mm^2) was mounted with its *c*-axis parallel to the φ axis of the goniostat. It was possible to measure 1899 reflexions (~97% of those accessible to Cu $K\alpha$ radiation) of which about 450 had a relative integrated intensity of 15–20 counts against a maximum of 182000 counts for reflexion $\bar{2}$02. These reflexions have been considered as 'unobserved' and treated as in the case of LMI.

Structure analysis and refinement

From a three-dimensional synthesis of the Patterson function it was possible to obtain approximate coordinates for the bromine atom and the six carbon atoms of the phenyl group. Two subsequent three-dimensional syntheses of electron density yielded a clear

Table 1. *Observed structure amplitudes and calculated structure factors* (*e*)

H	K	L	FO	FC
0	0	2	32.5	33.7
0	0	4	14.2	-14.0
0	0	8	10.7	-10.5
0	1	1	53.3	53.6
0	1	2	154.0	-164.4
0	1	3	26.4	25.7
0	1	4	39.2	-39.9
0	1	5	3.2	-3.3
0	1	6	17.3	-17.7
0	1	7	9.2	-9.5
0	1	8	7.9	-7.0
0	2	0	43.1	-40.1
0	2	2	12.6	-13.4
0	2	3	67.9	-66.5
0	2	4	25.1	22.9
0	2	5	33.5	-33.8
0	2	6	4.6	-5.3
0	2	7	15.5	-15.8
0	3	1	65.8	-65.1
0	3	2	31.4	-31.9
0	3	3	32.6	-32.5
0	3	4	42.9	-42.7
0	3	6	15.0	-15.0
0	3	7	8.3	8.4
0	3	8	4.1	-3.6
0	4	0	74.8	-76.3
0	4	1	22.1	-20.9
0	4	2	64.0	-65.2
0	4	4	5.2	-5.9
0	4	5	9.2	8.2
0	4	6	9.2	9.2
0	4	8	8.3	8.7
0	5	1	55.8	-59.4
0	5	2	13.3	14.2
0	5	4	26.9	26.5
0	5	6	11.6	11.6
0	5	7	5.6	5.9
0	6	0	20.7	-19.4
0	6	1	31.0	30.1
0	6	2	13.6	-13.1
0	6	3	48.3	49.9
0	6	4	9.5	8.5
0	6	5	15.6	19.4
0	6	6	6.9	-7.0
0	6	7•	3.5	11.3
0	7	1	41.3	41.9
0	7	2	32.9	34.0
0	7	3•	6.9	9.4
0	7	4	13.3	13.6
0	7	6	6.9	7.3
0	8	0	55.9	59.4
0	8	2	11.0	12.1
0	8	4	6.0	6.3
0	8	6	4.0	-3.8
0	9	1	26.4	27.6
0	9	2	11.6	-11.8
0	9	3	12.6	15.4
0	9	4	11.5	-11.6
0	9	6	5.4	-5.4
0	10	0	8.6	9.6
0	10	1	9.1	-9.8
0	10	2	4.3	-4.4
0	10	3	19.6	-20.6
0	10	5	12.2	-13.3
0	11	1	13.9	-15.6
0	11	2	8.4	-9.0
0	11	3	4.7	-5.5
0	11	4	6.7	-7.4
0	12	0	9.4	-11.4
0	12	2	10.5	-12.0
1	0	1	26.7	-24.1
-1	0	1	27.5	-26.1
1	0	3	49.4	-46.8
1	0	5	24.1	-23.8
-1	0	5	22.6	22.3
1	0	7	8.1	-6.1
-1	0	7	16.7	16.7
-1	0	9	4.3	4.1
1	1	0•	11.4	17.3
1	1	1•	14.0	-6.3
-1	1	1	25.5	29.0
1	1	2	99.3	-96.3
-1	1	2	76.2	-74.3
1	1	3	13.2	-12.0
-1	1	3	19.6	20.7
1	1	4	53.4	-51.9
-1	1	4	56.1	50.7
1	1	5	17.5	16.2
-1	1	5	20.5	20.5
1	1	6	15.8	-15.3
-1	1	6	22.0	22.6
1	1	7	7.4	7.9
-1	1	8	8.9	8.9
1	1	9	4.0	4.2
1	2	0	73.3	-80.3
1	2	1	15.4	-16.5
-1	2	1	6.6	6.9
1	2	2	51.9	-51.0
-1	2	2	93.0	92.4
1	2	3•	4.2	-5.7
-1	2	3	11.4	11.8
1	2	4	13.2	11.6
-1	2	4	67.3	68.5
-1	2	5	6.7	7.1
1	2	6	36.1	36.0
1	2	8	9.7	9.5
-1	2	8	8.2	-9.1
1	3	0	56.8	54.9
-1	3	1	57.5	59.5
1	3	2	32.2	33.5
-1	3	2	7.9	-6.7
-1	3	3	44.1	45.6
1	3	4	48.0	46.5
-1	3	4	19.1	-19.1
1	3	5	19.9	20.4
-1	3	5	13.5	12.5
1	3	6	6.0	5.5
-1	3	6	25.0	-25.4
1	3	7	11.6	11.9
-1	3	7	6.1	-7.1
1	3	8	3.8	-3.2
-1	3	8	3.9	-3.4
1	3	9•	4.0	5.7
1	4	0	10.5	-8.3
1	4	1	52.4	51.8
-1	4	1	21.5	21.6
1	4	2	12.0	-12.4
1	4	3	85.7	82.9
-1	4	3	22.5	-22.4
1	4	4	8.2	-7.5
-1	4	4	11.5	11.6
1	4	5	26.4	26.3
-1	4	5	41.5	-40.8
1	4	7	5.2	4.9
-1	4	7	14.6	-15.1
1	5	0	23.6	23.5
1	5	1	50.0	50.2
-1	5	1	60.4	-60.9
1	5	2	31.6	31.3
1	5	3	2.2	2.3
-1	5	3	41.5	-41.3
1	5	4	40.8	38.5
-1	5	4	11.3	-11.8
1	5	5	17.2	-17.0
-1	5	5	13.8	-13.7
1	5	6	12.9	13.1
-1	5	6•	12.3	-19.7
1	5	7	11.3	-11.7
-1	5	8	5.3	-4.5
1	6	0	45.6	46.8
1	6	1	9.3	-9.6
-1	6	1	7.3	8.3
1	6	2	24.5	23.6
-1	6	2	43.9	-45.2
1	6	3	7.9	-7.7
1	6	4	4.2	-4.6
-1	6	4	29.7	-28.9
1	6	6	16.1	-16.6
1	6	7	4.3	-4.5
1	6	8	6.0	-6.7
1	7	0	8.7	-10.2
1	7	1	10.3	8.8
-1	7	1	40.0	-41.3
1	7	2	37.3	-36.4
1	7	3	5.4	5.0
-1	7	3	21.4	-22.7
1	7	4	14.4	-14.1
-1	7	4	24.5	25.2
1	7	5	16.1	-16.8
-1	7	5	10.9	-11.1
1	7	6	5.8	-6.1
-1	7	6	6.8	4.9
1	7	7	6.1	-6.3
1	8	0	13.6	-13.6
1	8	1	34.3	-34.0
-1	8	1	15.1	-16.0
1	8	2	10.9	10.6
-1	8	2	12.3	13.4
1	8	3	38.5	-37.0
-1	8	3	15.1	15.6
-1	8	4	11.6	-12.6
1	8	5	16.4	-16.7
-1	8	5	18.4	18.4
-1	8	7	8.9	10.1
1	9	0	13.7	13.5
1	9	1	15.3	-16.0
-1	9	1	24.6	24.8
1	9	2	18.9	-18.1
-1	9	2	21.8	-22.2
1	9	3	3.5	-3.4
-1	9	3	17.6	18.4
1	9	4	12.5	-12.5
-1	9	4	6.0	7.1
1	9	5	11.8	11.2
1	9	6	4.4	-4.6
-1	9	6•	5.9	7.8
1	10	0	15.0	-15.1
1	10	1	2.9	-3.0
1	10	2	10.7	-10.9
-1	10	2	9.8	9.7
1	10	4	4.8	5.1
-1	10	4	14.4	15.9
1	11	1	7.9	-7.6
-1	11	1	15.1	14.9
1	11	2	11.8	11.4
-1	11	2	2.2	-2.5
-1	11	3	10.9	10.8
1	11	4	8.1	7.8
1	12	1	11.5	11.1
1	12	2	5.1	5.1
1	12	3	12.6	12.0
-1	12	3	5.8	-6.0
2	0	2	36.3	37.9
-2	0	2	227.9	-267.5
2	0	4	63.9	63.8
-2	0	4	52.2	-50.3
2	0	6	36.6	35.3
-2	0	6	9.1	-9.2
-2	0	8	13.8	13.2
2	1	0•	113.5	150.9
2	1	1	9.7	-10.9
-2	1	1	59.9	-58.1
2	1	2	89.0	86.5
-2	1	2	71.0	-71.3
2	1	3	26.6	19.2
-2	1	3	29.7	-29.5
2	1	4	30.6	29.6
-2	1	4	61.7	64.5
2	1	5	31.9	30.5
-2	1	5	18.5	-18.5
2	1	6	14.0	13.7
-2	1	7	10.9	10.8
2	1	7	4.8	-4.7
2	1	8	7.3	-7.8
-2	1	8	4.2	4.7
2	2	0•	8.3	-5.4
2	2	1	109.9	106.1
-2	2	1	34.1	-36.4
-2	2	2	6.7	6.5
2	2	3	15.6	15.5
-2	2	3	52.9	51.6
2	2	4	8.0	6.0
-2	2	4	22.8	23.4
-2	2	5	20.9	19.8
2	2	5	15.8	16.3
-2	2	6	16.9	-18.1
-2	2	7	7.8	-9.2
2	2	7	11.0	12.2
2	2	8	5.7	-6.6
-2	2	9•	5.4	7.1
2	3	0	80.4	80.9
-2	3	1	78.6	79.0
2	3	2	91.2	89.3
-2	3	2	17.3	-17.4
-2	3	3	17.0	-17.1
2	3	3	28.7	29.0
2	3	4	6.2	6.3
2	3	5	27.8	-26.6
-2	3	5	20.3	22.1
-2	3	6	6.3	5.3
2	3	7	17.2	-17.2
-2	3	7	5.6	5.3
2	3	8	5.2	-5.8
-2	3	9	7.9	9.4
2	4	0	62.4	62.4
-2	4	1	20.4	-19.3
2	4	1	15.3	-15.0
2	4	2	46.8	-42.7
-2	4	2	50.4	50.3
2	4	3	11.3	-9.4
-2	4	3	44.5	-40.8
2	4	4	39.4	39.2
-2	4	4	6.2	-6.5
2	4	5•	4.4	2.9
-2	4	6	21.9	-21.4
2	4	6	14.0	14.6
2	4	8	5.4	-5.8
2	5	0	29.6	-29.9
2	5	1	26.3	-24.3
-2	5	1	34.8	36.4
2	5	2	44.8	-42.9
-2	5	2	10.3	-12.1
2	5	3	18.7	-18.9
-2	5	3	41.9	41.6
2	5	4	8.0	-8.4
2	5	5	25.1	-24.1
-2	5	5	11.3	11.9
-2	5	6	9.2	-9.3
2	5	7	9.2	-9.5
-2	5	9	6.7	-6.9
2	6	0	12.5	12.5
2	6	1	65.1	-65.7
-2	6	1	57.2	57.7
2	6	2	12.1	-11.6
2	6	3	34.6	-33.6
-2	6	3	6.4	7.2
2	6	4	6.5	5.5
2	6	5	7.5	-7.9
2	6	6	19.5	-19.3
-2	6	7	5.8	-6.7
2	7	0	44.6	-45.4
2	7	1•	8.0	5.4
-2	7	1	26.4	-26.3
2	7	2	26.8	-27.0
-2	7	2	11.1	11.2
2	7	3	14.4	14.3
-2	7	3	33.9	-33.8
2	7	4	11.1	-10.3
-2	7	4	13.3	-14.4
2	7	5	17.7	17.7
-2	7	5	11.0	-11.9
2	7	6	7.1	-6.8
2	7	7	6.0	6.3
2	8	0	6.6	-6.3
2	8	1	5.7	-5.2
-2	8	1	6.0	-5.8
2	8	2	7.7	7.4
-2	8	2	47.1	-46.7
2	8	4	13.4	12.8
-2	8	4	9.2	-9.0
2	8	6	11.8	12.4
-2	8	6	6.6	-7.0
2	9	0	16.6	16.6
-2	9	1	20.4	-21.0
2	9	2	15.4	15.1
-2	9	2	8.7	-8.1
2	9	3	13.0	12.3
-2	9	3	17.6	-17.3
2	9	4	7.4	7.6
-2	9	4	6.6	6.8
2	9	5	15.4	15.3
-2	9	5	10.5	-10.7
-2	9	6	4.9	4.4
2	10	0	30.9	29.9
2	10	1	18.9	-18.9
-2	10	2	4.5	-5.1
2	10	3	20.2	19.8
2	10	5	5.1	5.3
-2	10	5	6.6	6.4
2	11	0	13.1	12.7
-2	11	1	12.1	13.1
2	11	2	14.1	13.2
-2	11	2	4.7	-4.6
2	11	3	5.3	-4.9
-2	11	3	9.9	10.5
2	12	0	9.6	8.7
2	12	2	6.2	-5.1
-2	12	2	9.1	8.6
3	0	1	51.3	54.2
-3	0	1	61.3	53.6
3	0	3	52.4	47.2
3	0	7	12.3	-12.4
3	0	9	6.5	-7.0
-3	0	9	5.4	-4.7
3	1	0	79.8	85.5
3	1	1	35.5	-31.4
-3	1	1	14.2	13.9
3	1	2	68.2	64.7
-3	1	2	44.6	45.1
3	1	3	38.3	-37.4
-3	1	3	18.3	-17.8
3	1	4	55.3	51.7
-3	1	5	16.0	-16.0
3	1	5	19.8	-19.9
-3	1	6	14.0	-13.8
3	1	6	13.2	-13.2
-3	1	7	9.9	-9.4
3	1	7	10.1	-9.7
3	1	8	7.6	-8.0
-3	1	8•	4.0	-6.0
3	2	0	17.9	-19.4
3	2	1•	3.5	6.2
3	2	2	64.0	-59.8
-3	2	2	18.9	-20.6
3	2	3	6.2	5.8
-3	2	3	13.5	-12.2
3	2	4	77.1	-74.6
-3	2	4	45.7	-45.3
3	2	5	7.1	7.6
3	2	6	19.5	-19.1
-3	2	6	37.0	-38.6
3	2	7	6.3	-6.7
-3	2	7	3.8	-3.6
-3	2	8	5.1	-4.5
3	3	0	45.8	-43.0
3	3	1	21.9	-20.4
-3	3	1	27.1	-26.9
3	3	2	56.1	-52.8
-3	3	2	54.7	-55.4
3	3	3	32.5	-32.1
-3	3	3	27.3	-28.2
3	3	4	9.6	7.9
-3	3	4	13.9	-14.3
3	3	5	27.2	-26.8
-3	3	5	24.4	-25.4
3	3	6	13.9	13.6
3	3	7	8.9	-9.0
-3	3	7	8.2	-8.3
-3	3	8	9.2	10.4
3	4	0	11.9	-9.4
3	4	1	87.4	-55.6
-3	4	1	56.1	-59.8
3	4	2	14.9	16.2
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-14	3	3	7.7	-8.0
-14	3	5	6.5	6.3
14	4	0	2.6	-2.5
14	4	2	3.5	-3.6
-14	4	2	5.7	7.3
-14	4	3	3.5	-3.6
14	5	0	8.7	-9.0
14	5	1	6.6	-6.1
14	5	2	4.6	-4.9
14	6	0	3.8	-4.3
14	6	1	11.5	-11.6
-14	6	1	5.2	6.1
15	0	1	7.2	6.4
-15	0	1	8.2	6.3
-15	0	3	9.2	9.4
15	1	0	6.6	6.6
15	1	1	6.3	-5.0
-15	1	1	8.2	4.5
-15	1	2	3.9	3.9
15	2	0	8.4	-7.9
15	2	2	10.1	-10.7
15	3	0	7.3	-6.6
15	3	1	5.1	-4.4
15	4	1	4.9	-5.9
16	0	0	11.0	-9.7
-16	0	2	4.4	-5.5

picture of the molecule, which appeared to be a furazan 5-oxide with all the atoms in very similar positions to those of the corresponding atoms of LMI, excepting the extranuclear oxygen atom of the furoxan ring. This atom is in fact bound to two different nitrogen atoms in the two isomers, which are therefore positional isomers.

For the refinement by the least-squares method we followed the same procedure described for LMI, as we did for the computation of atomic scattering factors and for the anomalous scattering correction. After refining only the coordinates and the scale factor, with an average vibrational parameter $B=3{\cdot}0$ Å^2, the value of R was $\sim 0{\cdot}15$ and after some isotropic cycles it was lowered to 0·116. The refinement with anisotropic vibrational parameters reduced R to 0·044 and the introduction and refinement of the positional parameters of the four hydrogen atoms of the benzene ring (obtained from a three-dimensional difference synthesis) yielded a final $R=0{\cdot}041$ (weighted $R=0{\cdot}047$). During the later cycles a few 'observed' reflexions, with abnormal Δ values were given zero weight; these are marked with an asterisk in the amplitudes table (Table 1), as are the values of the 'unobserved' reflexions with $|F_c| \gg |F_o|$. The final R value for all the reflexions listed in Table 1 is 0·053.

The final coordinates and vibrational anisotropic parameters (B_{ij} values) are reported in Table 2, with their standard deviations in units of the last significant figure. Concerning the influence of the lack of absorption correction on the estimated standard deviations, we can say, on the grounds of the work of Srivastava & Lingafelter (1966) and of Werner (1964), that they are certainly significant both for positional and thermal parameters. We point out that, as a result of the smaller dimensions of the HMI crystal with respect to those of LMI, for the former compound, we have found (with the same μ value and with intensities collected by the same procedure) better values of the e.s.d. and of R, so confirming the results of the above mentioned authors.

Description and discussion of the structure

The configuration of the HMI molecule is illustrated in Fig. 1, together with the numbering of its atoms. The molecular mean plane, referred to the crystallographic axes, has the following equation in fractional

Table 2. *Final fractional coordinates and vibrational parameters* (Å^2) *with, below, the significant figures of the standard deviations*

	x/a_0	y/b_0	z/c_0	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
C(1)	0·4162	0·2782	0·1409	3·69	3·83	4·17	−0·43	−0·28	0·22
	4	5	7	22	22	22	18	18	18
C(2)	0·5224	0·2678	0·1974	4·06	3·96	5·91	0·73	−1·27	−0·69
	4	5	7	23	22	29	18	22	20
C(3)	0·5761	0·3806	0·2561	3·08	4·61	6·26	0·51	−1·00	−0·85
	4	6	7	19	22	27	22	18	26
C(4)	0·5249	0·5016	0·2656	3·41	4·27	3·34	−0·01	0·05	0·28
	4	5	6	20	22	20	18	16	18
C(5)	0·4182	0·5064	0·2038	3·79	3·25	7·22	0·47	−0·67	0·58
	4	5	8	25	22	33	18	22	22
C(6)	0·3638	0·3952	0·1413	2·65	3·94	7·42	0·35	−0·79	0·24
	4	5	8	18	23	32	18	18	22
C(7)	0·5860	0·6169	0·3307	3·40	4·30	3·68	0·08	0·16	0·24
	3	5	6	18	21	20	20	14	20
C(8)	0·5517	0·7487	0·3492	4·41	4·05	3·93	−0·56	0·27	0·12
	4	5	7	23	22	22	18	18	18
C(9)	0·4466	0·8201	0·3131	5·81	4·02	9·58	1·57	−1·24	−1·05
	5	6	10	29	23	42	22	28	28
N(1)	0·6868	0·6041	0·3827	3·72	4·57	6·85	−0·14	−0·97	−0·08
	3	4	7	18	22	25	16	16	18
N(2)	0·6347	0·8157	0·4153	5·43	4·76	5·18	−0·86	−0·12	−1·06
	4	5	6	24	21	22	18	18	18
O(1)	0·7227	0·7278	0·4381	3·93	5·54	7·19	−1·14	−0·64	−0·37
	3	4	5	17	19	23	14	16	18
O(2)	0·6519	0·9326	0·4546	7·21	5·53	8·58	−2·15	0·49	−2·33
	4	4	7	25	20	27	20	22	20
Br	0·34074	0·12524	0·05357	4·84	4·03	5·88	−0·86	−1·16	0·23
	4	6	8	3	2	3	2	2	2
H(2)	0·561	0·183	0·205		$B=4{\cdot}0$ Å^2				
	5	6	7						
H(3)	0·660	0·384	0·293		$B=4{\cdot}0$				
	4	5	7						
H(5)	0·382	0·592	0·225		$B=4{\cdot}0$				
	4	6	7						
H(6)	0·289	0·403	0·123		$B=4{\cdot}0$				
	5	6	8						

coordinates:

$$3{\cdot}9859x+2{\cdot}0278y-7{\cdot}1321z=1{\cdot}2299\,. \qquad (1)$$

In Table 3, column I, the distances of the atoms of one molecule from this plane are reported. Assuming an average standard deviation of 0·008 Å, the molecule is possibly non-planar on the grounds of the χ^2 test; application of the t test reveals that atoms C(9) and O(2) are possibly out of plane (1). The mean planes for the bromophenyl and methylfuroxan groups have respectively the equations:

$$4{\cdot}0358x+2{\cdot}0068y-7{\cdot}1279z=1{\cdot}2446\,, \qquad (2)$$

$$3{\cdot}9215x+2{\cdot}0065y-7{\cdot}1451z=1{\cdot}1683\,. \qquad (3)$$

Table 3. *Distances* (Å) *of the molecular atoms from the reported planes*

	I	II	III
Br	−0·000	0·000	—
C(1)	0·011	0·011	—
C(2)	0·012	0·006	—
C(3)	−0·012	−0·019	—
C(4)	0·015	0·013	—
C(5)	−0·012	−0·007	—
C(6)	−0·014	−0·009	—
C(7)	0·002	—	−0·004
C(8)	0·003	—	−0·002
C(9)	0·019	—	0·008
N(1)	−0·003	—	−0·003
N(2)	0·008	—	0·010
O(1)	−0·002	—	0·004
O(2)	−0·018	—	−0·011
H(2)	0·085	0·076	—
H(3)	0·090	0·101	—
H(5)	0·112	0·119	—
H(6)	0·138	0·147	—

The distances of the atoms from planes (2) and (3) are listed in Table 3, columns II and III; the two parts of the molecule are planar, only atom C(3) is possibly out of plane (2).

Apart from slight differences due to the different position of the extranuclear oxygen atoms, the molecular packing of HMI, shown in Fig. 2, is the same as that of the lower melting isomer. The molecules are slightly inclined on plane (001) (~18°) and the two molecules related by a centre of symmetry face each other, as in LMI, *i.e.* in such a way as to superpose the least number of atoms; only atoms C(1), C(2) and C(6) (partially) of one molecule are superimposed respectively on atoms N(1), C(8) and O(1) of the related molecule; the distance between the facing benzene and furoxan rings is 3·58 Å and the same considerations hold for these molecules as for LMI.

Only one remarkable intermolecular contact occurs, *i.e.* that between the Br atom and the N(1) atom at $x-\frac{1}{2},\frac{1}{2}-y,z-\frac{1}{2}$ (3·23 Å).

As regards the molecular bond lengths and angles, reported in Table 4, the distribution of lengths in the phenyl group is analogous to that found in LMI, but now the value of the shortest bond, between C(1) and C(6), is significantly different from the longest, C(3)–C(4), and possibly different from the average length (1·381 Å). The explanation of these anomalies does not seem easy; anyway they are not uncommon in halogenophenyl compounds.

The double-bond character of C(4)–C(7) is of the same order of magnitude (~18%) as in LMI; also the trend of bond lengths in the furoxan ring is similar. However, in HMI the difference between N(1)–O(1) and N(2)–O(1) is smaller, even if still significant, while

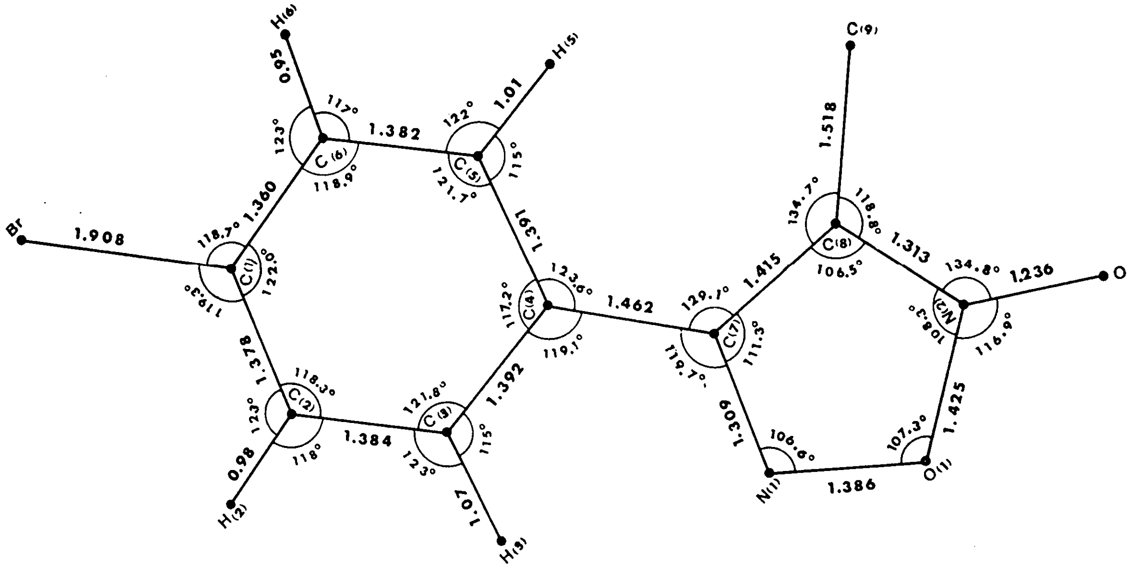

Fig. 1. Molecular bonds and angles.

Table 4. *Bond lengths* (Å) *and bond angles with the significant figures of the standard deviations in brackets*

Br—C(1)	1·908 (5) Å	C(7)-N(1)	1·309 (6) Å
C(1)-C(2)	1·378 (7)	C(8)-N(2)	1·313 (7)
C(2)-C(3)	1·384 (8)	N(1)-O(1)	1·386 (6)
C(3)-C(4)	1·392 (7)	N(2)-O(1)	1·425 (6)
C(4)-C(5)	1·391 (7)	N(2)-O(2)	1·236 (7)
C(5)-C(6)	1·382 (7)	C(2)-H(2)	0·98 (6)
C(6)-C(1)	1·360 (7)	C(3)-H(3)	1·07 (6)
C(4)-C(7)	1·462 (7)	C(5)-H(5)	1·01 (6)
C(7)-C(8)	1·415 (7)	C(6)-H(6)	0·95 (5)
C(8)-C(9)	1·518 (8)		
Br—C(1)-C(2)	119·3 (4)°	C(9)-C(8)-N(2)	118·8 (5)°
Br—C(1)-C(6)	118·7 (4)	C(7)-N(1)-O(1)	106·6 (4)
C(2)-C(1)-C(6)	122·0 (5)	C(8)-N(2)-O(1)	108·3 (4)
C(1)-C(2)-C(3)	118·3 (5)	C(8)-N(2)-O(2)	134·8 (5)
C(2)-C(3)-C(4)	121·8 (4)	O(1)-N(2)-O(2)	116·9 (4)
C(3)-C(4)-C(5)	117·2 (4)	N(1)-O(1)-N(2)	107·3 (3)
C(3)-C(4)-C(7)	119·1 (4)	H(2)-C(2)-C(1)	123 (3)°
C(5)-C(4)-C(7)	123·6 (4)	H(2)-C(2)-C(3)	118 (3)
C(4)-C(5)-C(6)	121·7 (5)	H(3)-C(3)-C(2)	123 (3)
C(5)-C(6)-C(1)	118·9 (5)	H(3)-C(3)-C(4)	115 (3)
C(4)-C(7)-C(8)	129·1 (4)	H(5)-C(5)-C(4)	115 (3)
C(4)-C(7)-N(1)	119·7 (4)	H(5)-C(5)-C(6)	122 (3)
C(8)-C(7)-N(1)	111·3 (4)	H(6)-C(6)-C(5)	117 (3)
C(7)-C(8)-C(9)	134·7 (5)	H(6)-C(6)-C(1)	123 (3)
C(7)-C(8)-N(2)	106·5 (4)		

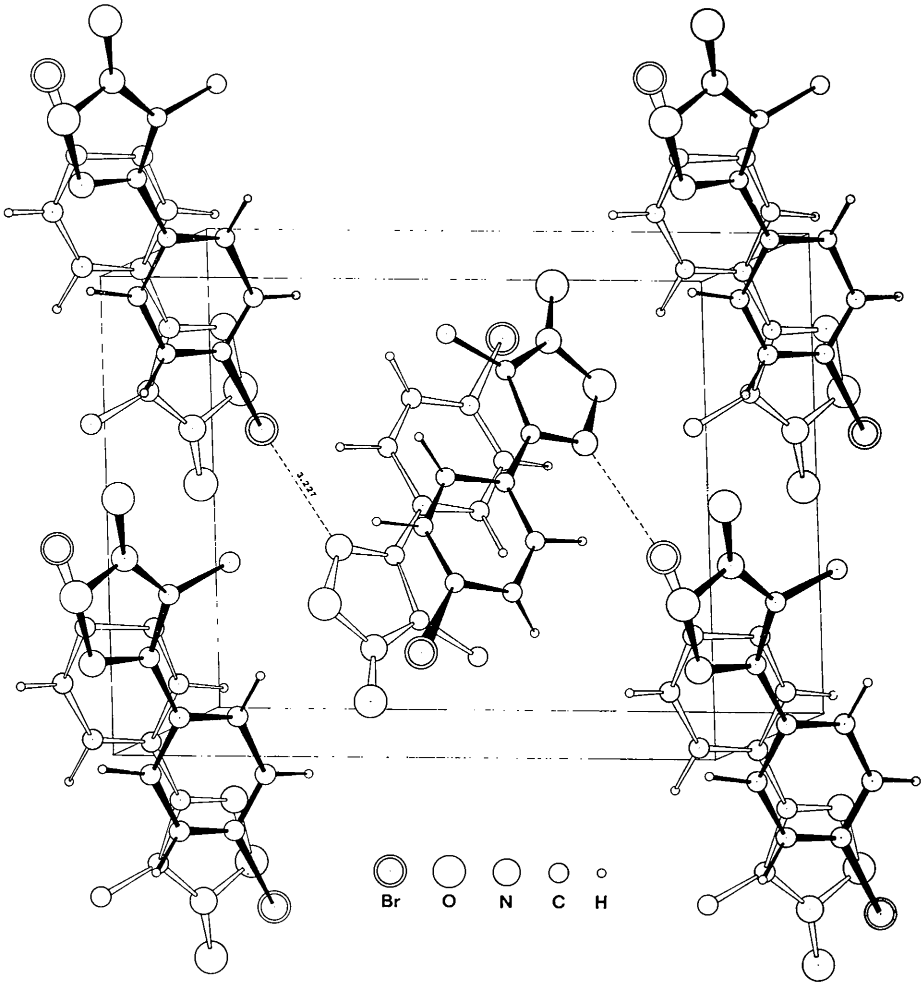

Fig. 2. Clinographic projection, along the z axis, of the contents of one unit cell (y axis vertical).

the difference between the two C=N bonds here is undoubtedly not significant.

In HMI the carbon atom of the methyl group is involved in two intramolecular contacts: with H(5) (2·52 ± 0·06 Å) and O(2) (2·950 ± 0·008 Å). These contacts may hinder, in the solid state, a hyperconjugation effect of CH_3, which is probably present in LMI; in fact the bond distance C(8)–C(9), in HMI, is only slightly shorter than that of a single bond.

In Table 5 are reported the elements characterizing the vibrational ellipsoids, referred to their own principal axes. All the considerations made on this subject for the lower melting isomer are valid also for the present compound. We point out that generally the thermal vibration in HMI is smaller than in LMI. This can be related either to the lower melting point of the latter compound or to the fact that, in the case of needle-crystals, the absorption effect artificially in-

Table 5. *Parameters characterizing the vibrational ellipsoids referred to their own principal axes*

	i	q_i (Å²)	r.m.s.d. (Å)	g_{i1}	g_{i2}	g_{i3}
C(1)	1	0·935	0·218	−0·163	0·807	−0·580
	2	1·214	0·248	−0·534	0·412	0·690
	3	0·802	0·202	0·829	0·424	0·433
C(2)	1	0·947	0·219	0·239	0·869	0·452
	2	1·842	0·305	0·471	0·286	−0·791
	3	0·766	0·197	−0·849	0·403	−0·412
C(3)	1	1·064	0·232	0·003	0·928	0·370
	2	1·825	0·304	0·308	0·352	−0·854
	3	0·660	0·183	−0·951	0·117	−0·365
C(4)	1	0·896	0·213	0·774	0·249	−0·514
	2	1·090	0·235	−0·087	0·952	0·284
	3	0·779	0·199	−0·627	0·176	−0·810
C(5)	1	0·996	0·225	0·787	0·602	0·200
	2	1·927	0·312	−0·236	0·093	0·944
	3	0·690	0·187	−0·570	0·793	−0·263
C(6)	1	1·006	0·226	0·238	0·971	0·031
	2	1·958	0·315	−0·191	0·036	0·961
	3	0·589	0·173	−0·952	0·235	−0·274
C(7)	1	0·923	0·216	0·432	0·269	−0·821
	2	1·092	0·236	0·039	0·948	0·318
	3	0·832	0·205	−0·901	0·170	−0·474
C(8)	1	0·982	0·223	0·304	0·092	0·971
	2	1·214	0·248	−0·786	0·587	0·127
	3	0·905	0·214	0·540	0·804	−0·202
C(9)	1	1·419	0·268	0·788	0·427	0·509
	2	2·736	0·372	0·376	0·238	−0·860
	3	0·775	0·198	−0·488	0·872	−0·014
N(1)	1	1·147	0·241	−0·112	0·993	−0·040
	2	1·882	0·309	0·321	0·008	−0·916
	3	0·816	0·203	0·940	0·116	0·398
N(2)	1	1·485	0·274	−0·822	0·110	0·487
	2	1·520	0·278	−0·418	0·706	−0·606
	3	0·863	0·209	0·464	0·707	0·570
O(1)	1	1·525	0·278	−0·417	0·900	−0·157
	2	1·909	0·311	−0·258	0·011	0·940
	3	0·776	0·198	0·871	0·435	0·301
O(2)	1	1·975	0·316	−0·804	0·226	0·480
	2	2·518	0·357	−0·369	0·536	−0·788
	3	0·845	0·207	0·467	0·814	0·385
Br	1	1·090	0·235	−0·462	0·712	−0·566
	2	1·843	0·306	−0·569	0·219	0·741
	3	0·824	0·204	0·680	0·667	0·360

creases the thermal motion with increase in length of the needle (the LMI crystal was longer than that of the HMI), as stated by Srivastava & Lingafelter (1966).

Comparison of the structures of the two isomers

As outlined in the work on LMI, the problems regarding the isomerism of aryl-alkyl furoxans are of two kinds; the type of isomerism and the different chemical behaviour of the isomers. The former problem can be considered as solved by the present X-ray structural analysis, while the latter requires some other physical-chemical studies.

The following chemical properties of aryl-alkyl furoxans have to be considered. According to Ponzio (1928*a*,*b*) only one isomer reacts with PCl_5 giving the corresponding furazan and undergoes the isoxazolinic rearrangement with EtNa. Boulton, Katrizky & Hamid (private communication) have studied the thermal interconvertibility of these isomers, which at equilibrium yield 1·6 parts of one isomer against 1·0 of the other; this last property is explained by the formation of an intermediate dinitroso compound. We remember, incidentally, that condensed aromatic furoxans do not present isomers and this fact can be explained by assuming an easy tautomerism *via* a dinitroso intermediate compound.

As mentioned above, among our two isomers, the LMI is the more stable on the basis of the above chemical considerations.

Now, the most interesting difference between corresponding bond lengths in our isomers is that in the distances C(8)–C(9); this bond is significantly longer in HMI than in LMI, while, considering the reactivity of the former compound towards EtNa, one should expect a more marked hyperconjugation from the methyl group for the former isomer. A calculation of bond orders made by Hückel's method also predicts a shorter C(8)–C(9) bond for HMI. This anomaly can be explained by supposing that in HMI the two intramolecular contacts involving the methyl group, and especially that with the extranuclear oxygen atom, lead to an arrangement unsuitable for hyperconjugation (*cf.* also the values of bond angles), while in LMI the methyl group is involved in only one weaker contact. A very interesting feature of this latter compound is the interaction O(2)- - -H(3)–C(3), which leads to the formation of a six membered ring and can explain the lack of reactivity of LMI towards PCl_5. This interaction can also explain the preference shown by naphthofuroxans for tautomeric forms like that of our LMI (Boulton & Clifford, private communication). In general we can say that the trend of bond distances in our furoxan rings is quite similar to that found in benzofuroxans (Britton & Noland, 1962; Kamenar & Prout, 1965; Cady, Larson & Cromer, 1966).

On the basis of the above considerations, it seems reasonable to infer that in aryl-alkyl furoxans the 2-oxide form corresponds to the more stable isomer, while the 5-oxide form corresponds to the less stable. Of course the melting points are not necessarily criteria of structure, but, in most cases, as in ours, we have seen that the lower melting isomers have the properties of the more stable 2-oxide form and the higher melting isomers behave as the less stable 5-oxide form.

The computations were done by Olivetti ELEA 6001 and IBM 7090 (C.N.U.C.E., Pisa) computers.

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