lization is an essentially planar backbone with maximum departures from *syn* and *anti* geometry of *ca* 10°.

There is an intramolecular hydrogen bond (2·84 Å) between N(1) and O(2) [H(1)···O(2) 2·11 Å, N—H···O angle 130°]. Symmetry-related molecules are linked *via* N—H···O hydrogen bonds (Fig. 2) between the amine N and sulfone O atoms to form continuous chains in the crystal.

Despite certain unfavourable characteristics, the overall geometry of (1), in particular the spatial relationship of N(1) and O(2), indicates a potential for chelate coordination to one or two metal atoms with retention of planarity within the ligand.

We wish to thank Dr J. Michael, Hoechst UK, for supplying the original sample of (1).

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Structure of 2-Amino-1-(*p*-methoxyphenyl)-4-imidazolecarbaldehyde

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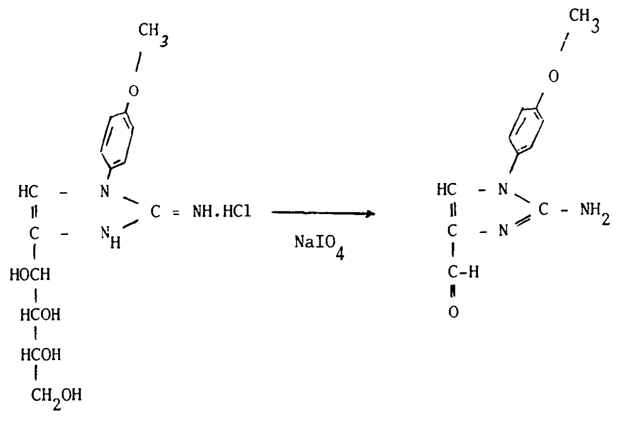
Abstract. $C_{11}H_{11}N_3O_2$, $M_r = 217{\cdot}2$, triclinic, $P\bar{1}$, $a = 8{\cdot}020\,(2)$, $b = 8{\cdot}490\,(4)$, $c = 9{\cdot}031\,(4)$ Å, $\alpha = 117{\cdot}19\,(6)$, $\beta = 102{\cdot}66\,(4)$, $\lambda = 72{\cdot}22\,(4)°$, $V = 518{\cdot}4\,(5)$ Å^3, $Z = 2$, $D_x = 1{\cdot}39$, $D_m = 1{\cdot}40$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}9$ cm^{-1}, $F(000) = 228$, room temperature, final $R = 0{\cdot}06$ for 1329 observed reflections. The dihedral angle between the imidazole plane and the aromatic ring is 55·3 (1)°. The double bonds in the imidazole ring are delocalized. The molecules are linked by van der Waals forces, although there is one short contact between the N(amino) and the O(carbonyl) atoms.

Introduction. This is one of a series of new imidazole derivatives that we are investigating. We have previously determined the crystal structures of 2-amino-3-methyl-5-(D-*arabino*-1,2,3,4-tetrahydroxybutyl)imidazolium chloride (Vega, López-Castro & Márquez, 1988) and 2-amino-1-methyl-4-imidazolecarbaldehyde (Pérez-Garrido, Moreno, Criado & López-Castro, 1988). The title compound (II) has been synthesized at the Organic Chemistry Department of Seville University by Professor Fdez-Bolaños and co-workers by oxidation with $NaIO_4$ of 2-amino-3-(*p*-methoxyphenyl)-5-(D-*arabino*-1,2,3,4-tetrahydroxybutyl)imidazolium chloride (I).



(I) (II)

The compound, as with other analogues, has been studied by UV, IR and NMR (Alaiz-Barragán, 1987), and the crystal-structure determination of the title compound was undertaken in order to establish possible correlations with the spectroscopic data. The resolution of the structure confirms the molecular conformation and the canonical form that contributes most to the structure, as shown by the spectroscopic data.

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Experimental. Crystal size 0·39 × 0·28 × 0·20 mm. Density measured by flotation. Enraf–Nonius CAD-4 diffractometer with graphite monochromator and Mo $K\alpha$ radiation. Cell dimensions from 2θ angles for 25 reflections ($5 < \theta < 14°$). $\omega/2\theta$ mode, $2\theta_{\max} = 45°$ ($0 \le h \le 10$, $-10 \le k \le 10$, $-12 \le l \le 12$). From 1437 independent reflections measured, only 1329 were considered as observed, $R_{\rm int} = 0{\cdot}005$ from merging 28 equivalent reflections, $I > 2\sigma(I)$; Lp correction, absorption ignored; two check reflections (333, $\overline{3}\overline{3}\overline{3}$) every 5400 s showed no unusual variation; direct methods, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); full-matrix least-squares refinement based on F, anisotropic temperature factors for the non-H atoms; difference Fourier synthesis revealed H atoms which were included in fixed positions with a common $U_{\rm iso}$ value. Further least-squares refinement gave $R = 0{\cdot}06$ ($wR = 0{\cdot}08$) ($R_{\rm intensities} = 0{\cdot}09$), weighting scheme based on statistical count criterion $w = 1/\sigma^2(F)$. $(\Delta/\sigma)_{\max} = 0{\cdot}01$ for non-H atoms, $S = 2{\cdot}55$ for 145 refined parameters. Nine reflections/parameter. Final difference synthesis showed $\Delta\rho = \pm 0{\cdot}5$ e Å^{-3}. Neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974). Crystallographic programs in *XRAY*70 system (Stewart, Kundell & Baldwin, 1970) were used.

Discussion. Table 1 gives the atomic coordinates and Table 2 the bond lengths and angles.* A view of the molecule with the atom numbering is shown in Fig. 1.

The molecule has two planar parts: the imidazole ring and the methoxyphenyl group [maximum deviation 0·004 (2) and 0·015 (3) Å respectively]. The substituents N3, C5, C4 and O1 are −0·017 (2), −0·109 (2), −0·034 (3) and −0·121 (2) Å out of the imidazole plane. The dihedral angle between the imidazole ring and methoxyphenyl group is 55·3 (1)°.

The C=O bond length is normal at 1·233 (5) Å [*International Tables for X-ray Crystallography* (1962): 1·23 (1) Å] and the shortened C9—O2 bond at 1·357 (4) Å shows the influence of the aromatic ring [*International Tables for X-ray Crystallography* (1962): 1·36 (1) Å]. The shortened C2—C4 bond [1·448 (3) Å] linking the C=O and C=C double bonds shows some multiple-bond character. C1—N2 at 1·326 (2) Å is shorter than C1—N3 at 1·359 (2), C1—N1 at 1·382 (3), C3—N1 at 1·390 (2) and N2—C2 at 1·388 (2) Å. The values are all intermediate between double- (1·265 Å) and single-bond

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

$U_{\rm eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j\cos(\mathbf{a}_i\mathbf{a}_j)$.

	x	y	z	$U_{\rm eq}$
O1	15179 (2)	3089 (3)	569 (2)	66 (2)
O2	6499 (3)	956 (2)	5458 (3)	62 (2)
N1	10562 (2)	2402 (2)	2177 (2)	43 (2)
N2	11514 (2)	3652 (2)	905 (2)	44 (2)
N3	8433 (2)	4466 (2)	1157 (2)	57 (2)
C1	10114 (2)	3551 (2)	1382 (2)	42 (2)
C2	12913 (2)	2520 (2)	1425 (2)	41 (2)
C3	12376 (3)	1784 (3)	2190 (2)	46 (2)
C4	14717 (2)	3370 (4)	1179 (3)	49 (2)
C5	9443 (2)	2056 (3)	2979 (2)	43 (2)
C6	9431 (3)	270 (2)	2584 (2)	46 (2)
C7	8415 (3)	−52 (3)	3444 (4)	51 (2)
C8	7417 (3)	1421 (3)	4684 (2)	45 (2)
C9	7395 (3)	3200 (3)	5024 (3)	48 (2)
C10	8421 (3)	3517 (3)	4186 (3)	48 (2)
C11	5403 (5)	2449 (5)	6716 (4)	69 (3)

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

O2—C8	1·357 (4)	C8—C9	1·392 (4)
O2—C11	1·453 (4)	C10—C9	1·384 (5)
N1—C5	1·434 (3)	C4—C2	1·448 (3)
N1—C1	1·381 (3)	C4—O1	1·233 (5)
N1—C3	1·390 (3)	N3—C1	1·359 (2)
C5—C10	1·390 (3)	C2—N2	1·387 (2)
C5—C6	1·392 (3)	C2—C3	1·354 (3)
C7—C8	1·400 (3)	N2—C1	1·326 (2)
C7—C6	1·396 (4)		

C8—O2—C11	116·5 (3)	C2—C4—O1	124·2 (3)
C1—N1—C3	106·6 (2)	C8—C9—C10	120·0 (3)
C5—N1—C3	125·0 (2)	C5—C6—C7	119·4 (2)
C5—N1—C1	128·1 (2)	C4—C2—C3	125·6 (3)
N1—C5—C6	119·9 (2)	C4—C2—N2	122·4 (2)
N1—C5—C10	119·2 (3)	N2—C2—C3	111·9 (2)
C10—C5—C6	120·7 (2)	C2—N2—C1	104·4 (2)
C8—C7—C6	119·6 (3)	N3—C1—N2	125·4 (2)
O2—C8—C7	114·9 (3)	N1—C1—N2	111·7 (2)
C7—C8—C9	120·2 (2)	N1—C1—N3	122·8 (2)
O2—C8—C9	124·9 (2)	N1—C3—C2	105·3 (2)
C5—C10—C9	119·9 (3)		

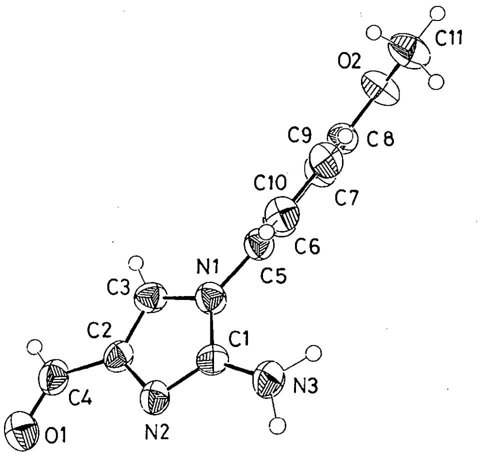

Fig. 1. *ORTEP* view (Johnson, 1965) of the molecule along the *a* axis, showing the atomic numbering.

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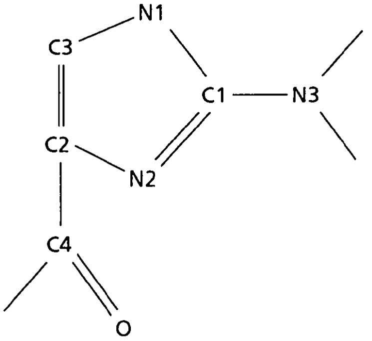
* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52712 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

(1·470 Å) values. The C2—C3 bond at 1·354 (3) Å is also intermediate between a double (1·330 Å) and a single C—C bond (1·541 Å). These results indicate, as in other aminoimidazole derivatives (Vega *et al.*, 1988; Pérez-Garrido *et al.*, 1988), some electronic delocalization in the imidazole ring and a major contribution from the following resonance structure:



Crystal packing is governed by van der Waals contacts, although there is one short contact, N3—H···O1($x-1, y, z$) = 3·025 (3) Å (N—H···O angle 142°), which may be a weak intermolecular hydrogen bond.

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The Structure of [(4-Nitrophenyl)methyl]triphenylphosphonium Bromide Methanol Solvate

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Abstract. $C_{25}H_{21}NO_2P^+.Br^-.2{\cdot}2CH_3OH$, M_r = 548·8, monoclinic, $C2/c$, a = 20·794 (2), b = 18·899 (2), c = 14·547 (1) Å, β = 107·55 (1)°, V = 5450·7 (9) Å^3, Z = 8, D_x = 1·337 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 15·8 cm^{-1}, $F(000)$ = 2268·8, R = 0·048 for 2815 observed [$I \geq 2{\cdot}5\sigma(I)$] unique reflexions measured at 295 K. The methanol molecules are found as an inhomogeneous electron density inside a continuous channel in the **c** direction. Through this channel, formed by hydrophobic phenyl groups, the loosely bound hydrophilic methanol molecules can easily escape from the crystal, resulting in the observed rapid disintegration of the crystals when removed from the mother liquor. The contribution of the disordered methanol molecules to the calculated structure factor is determined using a special method based on direct Fourier transformation of the observed electron density. The phenyl rings of the title compound are in a propeller configuration around the P atom. The C—C bond lengths in the phenyl groups are on average 0·016 (4) Å shorter for the bonds far from the P atom compared to the bonds near this atom.

Introduction. Crystals of the title compound could be obtained from several solvents. The crystals from

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