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CRYSTAL AND MOLECULAR STRUCTURE OF 2-METHYLBENZIMIDAZOLE

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In order to study the structures of the products of solid state catalytic condensation of o-diaminobenzene with acetate in the presence of I_2 (190-200°, 200-250° atm) in an inert gas medium we have carried out an x-ray structural investigation of one of these products viz. 2-methylbenzimidazole (I) (autodiffractometer CAD-4-SDP-55t, Mo Kα radiation, ω/4/3 θ-scan, θ_{max} = 30°). Crystals of I were tetragonal, a = 13.950(9), b = 7.192(3) Å, Z = 8, space group $P4_2/n$. The structure was solved by direct methods. The H atoms were located by difference Fourier synthesis. The H(N) atom was measured in two positions (H(NI) and H(N2)) with 0.54 and 0.46 occupancies. Anisotropic-isotropic (H) refinement (633 reflections with $I \geq 3\sigma$, unit weights, inclusion of secondary extinction) was carried out to R = 0.059, R_w = 0.52. Atomic coordinates are given in Table 1, bond lengths and bond angles in Fig. 1.

The bicyclic system of I is planar. The torsion angles do not exceed 0.8(6)° in the imidazole ring and 1.4(8)° in the benzene ring where the maximum deviation from this plane (C(3)) is 0.024 Å. The methyl group at atom C(8) deviates from the plane of the bicyclic system at 0.054 Å.

As a result of partial protonation of both nitrogen atoms in two positions (statistical distribution of H(N) atom referred to above) the N(1)–C(2) and N(2)–C(2) bond lengths are equal (see Fig. 1) as can be seen in the imidazoline cation [1]. The crystal structure of I can be regarded as a superposition of two tautomeric forms (see top of following page);

TABLE 1. Coordinates of Nonhydrogen Atoms (×10⁴), H Atoms (×10³) and Temperature Factors

Atom	x	y	z	B*
N(1)	2923(2)	1566(2)	69(6)	3.55(8)
N(2)	4024(2)	413(2)	−82(7)	4.26(9)
C(1)	2466(3)	703(3)	443(7)	3.43(9)
C(2)	3844(3)	1348(3)	−250(6)	3.33(9)
C(3)	3159(3)	−17(3)	354(8)	3.9(1)
C(4)	2897(4)	−967(3)	620(10)	5.8(1)
C(5)	1959(4)	−1164(4)	970(10)	6.4(2)
C(6)	1268(4)	−443(4)	1081(8)	4.9(1)
C(7)	1514(3)	505(4)	797(7)	4.5(1)
C(8)	4589(3)	2076(3)	−715(8)	4.4(1)
H(N1)	267(7)	211(5)	−10(10)	4(1)
H(N2)	456(7)	13(8)	−40(20)	4(1)

*Given here are B_{equi} values for anisotropically refined atoms in the form $B_{equi} = 4/3[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab\cos\gamma B(1,2) + ac\cos\beta B(1,3) + bc\cos\alpha B(2,3)]$ and B_{iso} for H(N) atoms.

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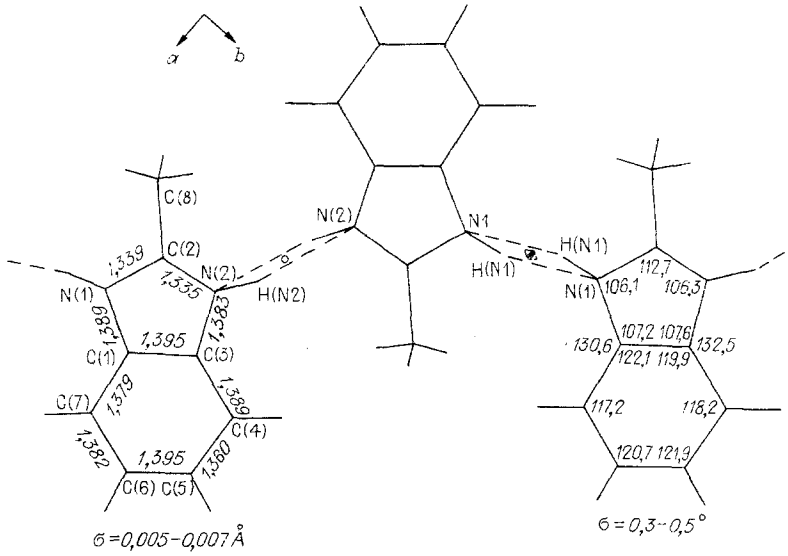
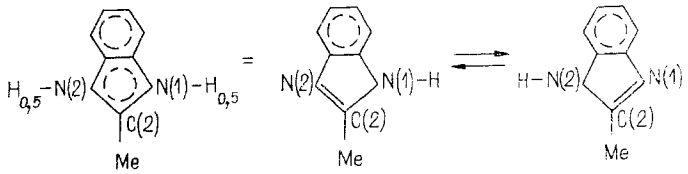


Fig. 1. Structure of the chain in Crystal I (projection on the ab plane).



In those benzimidazole and imidazole molecules where the H(N) atom is fixed at one of the two nitrogen atoms the C–N bond lengths differ: 1.361(7), 1.315(8) [2, 3] and 1.337(3), 1.316(2) Å [4, 5], respectively.

In structure I we found two intermolecular hydrogen bonds (HB): N(1)–H(N1)...N(1) [N(1)...N(1) 2.861(5), H(N1)...N(1) 2.04(8) Å, angle at the H(N1) atom 168(3)° and N(2)–H(N2)...N(2) 2.960(5), H(N2)...N(2) 2.13(10) Å angle at the H(N2) atom 178(8)°]. As a result the HB molecules linked by the twofold axes at [1/4, 1/4, z] and the centers of symmetry at 1/2 0 0 give rise to chains in the [202] direction (see Fig. 1).

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