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BENZIMIDAZOL, $C_7H_6N_2$.

C.J. Dik-Edixhoven, H. Schenk and H. van der Meer.*

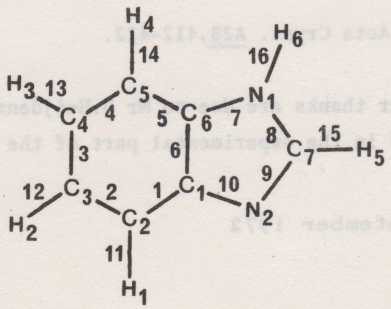
Laboratory for Crystallography, University of Amsterdam

Nieuwe Prinsengracht 126, Amsterdam, The Netherlands.

Preliminary information. The crystal structure of benzimidazol was solved as part of a study of several imidazol derivatives aimed at the geometry of the molecule and the hydrogen bonds between them.

Crystal data. Cell constants obtained from Weissenberg photographs calibrated with Al-powder lines : a = 6.940 (1), b = 13.498 (1), c = 6.808 (1), Z = 4, space group $P2_1nb$ (33)

Intensity data, structure determination and refinement. Intensities of 609 reflections were measured using a Nonius single crystal diffractometer with Ni-filtered CuK-radiation up to θ = 68.5° and operating in θ -2θ scan-mode. After an unsuccessful trial to solve the crystal structure from the Patterson function, it was solved by the sigma P-method (Schenk, 1972). The coordinates of the hydrogen atoms were found from a difference synthesis. Full matrix refinement (CRYLSQ) with anisotropic temperature factors for the carbon and nitrogen atoms and isotropic ones for hydrogen yielded a final R index of 0.040.



Fractional Atomic coordinates ($x10^4$).

	x	σ	y	σ	z	σ		x	σ	y	σ	z	σ
C(1)	2168	(0)	1356	(2)	0101	(4)	H(1)	4212	(63)	0392	(24)	-0671	(54)
C(2)	3405	(6)	0560	(2)	0385	(5)	H(2)	4371	(56)	-0441	(25)	2440	(51)
C(3)	3343	(7)	0079	(3)	2184	(5)	H(3)	2436	(77)	0067	(35)	5049	(71)
C(4)	2068	(7)	0388	(3)	3657	(4)	H(4)	-0013	(60)	1396	(24)	4475	(54)
C(5)	0829	(7)	1175	(2)	3406	(4)	H(5)	-0048	(57)	3115	(26)	-1908	(50)
C(6)	0895	(6)	1645	(2)	1573	(4)	H(6)	-1085	(65)	2754	(24)	1418	(47)
C(7)	0537	(7)	2572	(2)	-1023	(4)							
N(1)	-0128	(6)	2425	(2)	0811	(4)							
N(2)	1912	(6)	1959	(2)	-1542	(3)							

Bond distances and angles.

1 = 1.389(4) Å	6 = 1.392(4) Å	11 = 0.94(4) Å
2 = 1.386(4)	7 = 1.372(4)	12 = 1.02(4)
3 = 1.401(5)	8 = 1.346(4)	13 = 1.07(4)
4 = 1.378(5)	9 = 1.311(5)	14 = 0.98(4)
5 = 1.401(4)	10 = 1.395(3)	15 = 1.03(4)
		16 = 0.90(4)

1,2 = 117.8(3)°	5,7 = 131.9(3)°	1,11 = 117(2)°	4,14 = 121(2)°
1,6 = 120.6(3)	6,7 = 105.8(2)	2,11 = 126(2)	5,14 = 123(2)
1,10= 130.0(2)	6,10= 109.5(2)	2,12 = 117(2)	7,16 = 126(2)
2,3 = 120.9(3)	7,8 = 106.6(3)	3,12 = 122(2)	8,16 = 127(2)
3,4 = 122.3(3)	8,9 = 114.0(3)	3,13 = 111(3)	8,15 = 121(2)
4,5 = 116.1(3)	9,10= 104.2(2)	4,13 = 125(3)	9,15 = 125(2)
5,6 = 122.4(3)			

Comments. All atoms are within two times their positional standard deviation in the plane defined by the carbon and nitrogen atoms. Each molecule is connected with two neighbours, generated by a twofold screw axis along the x-axis, via a hydrogen bond of 2.00(4) Å from H(6) to N(2)'.

Reference.

Schenk, H.,(1972), Acta Cryst. A28,412-422.

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