Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\times 10^3$) *with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$. The e.s.d. for U_{eq} is the mean of those for the diagonal elements of U_{ij}.

	x	y	z	U_{eq}(Å^2)
O	1142 (3)	11606 (3)	5605 (3)	42 (2)
N	433 (3)	9692 (3)	6984 (3)	33 (2)
C(1)	2387 (4)	11136 (4)	8104 (4)	40 (2)
C(2)	3793 (5)	11478 (7)	8105 (6)	61 (3)
C(3)	4476 (5)	10245 (8)	7495 (6)	73 (4)
C(4)	3660 (5)	9773 (7)	5963 (6)	63 (3)
C(5)	2305 (4)	9250 (4)	6049 (5)	43 (2)
C(6)	1568 (3)	10459 (4)	6646 (4)	30 (2)
C(7)	−211 (4)	10561 (5)	7940 (5)	44 (2)
C(8)	799 (4)	9476 (5)	8637 (4)	42 (2)
C(9)	2176 (5)	10060 (5)	9288 (4)	48 (3)

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

C(1)—C(2)	1·517 (7)	C(6)—O	1·403 (4)
C(1)—C(6)	1·533 (6)	C(6)—N	1·486 (5)
C(1)—C(9)	1·528 (6)	N—C(7)	1·479 (5)
C(2)—C(3)	1·510 (9)	N—C(8)	1·504 (5)
C(3)—C(4)	1·524 (8)	C(7)—C(8)	1·460 (7)
C(4)—C(5)	1·529 (7)	C(8)—C(9)	1·514 (6)
C(5)—C(6)	1·522 (5)		
C(2)—C(1)—C(6)	113·7 (4)	N—C(6)—C(5)	105·8 (3)
C(2)—C(1)—C(9)	117·3 (4)	C(1)—C(6)—C(5)	112·5 (4)
C(6)—C(1)—C(9)	103·9 (3)	C(6)—N—C(7)	114·5 (3)
C(1)—C(2)—C(3)	114·8 (5)	C(6)—N—C(8)	106·0 (3)
C(2)—C(3)—C(4)	110·5 (5)	C(7)—N—C(8)	58·6 (3)
C(3)—C(4)—C(5)	109·8 (5)	N—C(7)—C(8)	61·6 (3)
C(4)—C(5)—C(6)	112·4 (4)	N—C(8)—C(7)	59·9 (3)
O—C(6)—N	110·8 (3)	N—C(8)—C(9)	109·1 (3)
O—C(6)—C(1)	109·4 (3)	C(7)—C(8)—C(9)	117·5 (4)
O—C(6)—C(5)	111·3 (3)	C(1)—C(9)—C(8)	103·4 (4)
N—C(6)—C(1)	106·8 (3)		

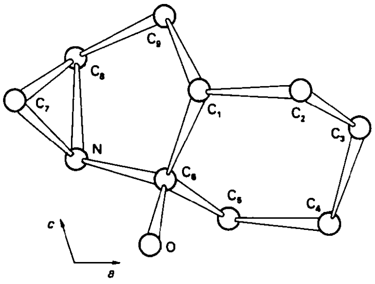

Fig. 1. Projection of the molecule showing the numbering of the atoms.

and a scale factor were refined by full-matrix least-squares calculations based on F and with unit weights. H atoms located on a difference map and included in refinement with isotropic thermal parameters. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Final $R = 0{\cdot}059$ and $wR = 0{\cdot}061$ for 100 parameters and 929 reflexions. $(\Delta/\sigma)_{\max} = 0{\cdot}4$, $\Delta\rho = -0{\cdot}3$ to $0{\cdot}4$ e Å^{-3}. Fig. 1. is a projection of the molecule showing the numbering of the atoms, coordinates are listed in Table 1, bond distances and angles are given in Table 2.* Computer programs used: *DATAP* and *DSORTH* (State University of New York, Buffalo) – data processing; modified *ORFLS* (Busing, Martin & Levy, 1962) – least-squares refinement; *ORTEP* (Johnson, 1965) – bonds and angles.

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Structure of 5,6-Dimethylbenzimidazole

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Abstract. $C_9H_{10}N_2$, $M_r = 146{\cdot}19$, monoclinic, $P2_1/c$, $a = 6{\cdot}513$ (2), $b = 27{\cdot}794$ (6), $c = 14{\cdot}058$ (2) Å, $\beta = 102{\cdot}62$ (2)°, $V = 2483{\cdot}3$ Å^3, $Z = 12$, $D_m = 1{\cdot}17$, $D_x = 1{\cdot}173$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}67$ cm^{-1}, $F(000) = 936$, $T = 298$ K, final $R = 0{\cdot}045$ for 2962 observed reflections. There are three crystal-

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lographically independent, but practically identical, molecules. They present very similar structural parameters for chemically equivalent bonds. There are no unusual bond distances or angles. In each molecule all atoms are essentially coplanar. The three crystallographically independent molecules are linked through hydrogen bonds involving N—H···N; this motif is repeated along the c axis to form an infinite molecular chain.

Experimental. D_m measured by flotation in a solution of CCl_4 and cyclohexane. A prismatic semi-transparent crystal ($0{\cdot}10 \times 0{\cdot}38 \times 0{\cdot}62$ mm) was mounted on a glass fiber. Cell constants from a least-squares fit to the angular settings of 25 reflections with $11{\cdot}53 < \theta < 14{\cdot}04°$ measured on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator. Systematic absences $0k0$ for k odd, $h0l$ for l odd indicate the space group $P2_1/c$. Intensity data collected with Mo radiation in an ω-scan mode: scan range $\Delta(\omega) = (0{\cdot}60 + 0{\cdot}35\tan\theta)°$, variable scan speed with max. $4{\cdot}12°\ \text{min}^{-1}$ and min. $1{\cdot}03°\ \text{min}^{-1}$. Four standard reflections measured every hour, no systematic change observed (1·0% variation over 47·1 h radiation time). Data corrected for Lorentz–polarization effects but not for absorption. 6297 reflections ($0 < h < 8$, $0 < k < 36$, $-18 < l < 18$) collected for monoclinic lattice, $4 < 2\theta < 54{\cdot}90°$, Friedel pairs averaged, agreement factors 0·032 on F_o, leaving 5670 unique reflections. 2962 observed reflections with $I < 3\sigma(I)$. Structure solved by direct method using *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978).

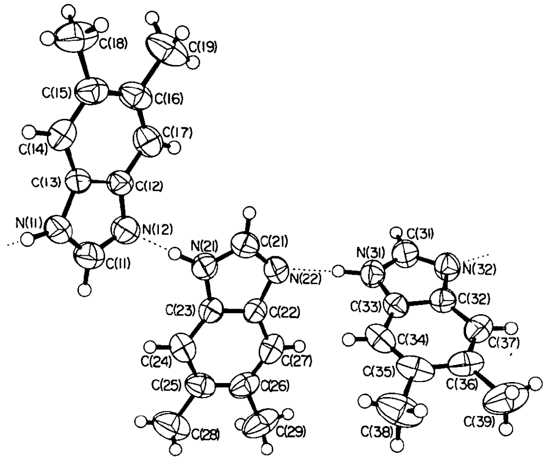

Fig. 1. *ORTEP*II drawing (Johnson, 1976) of the three crystallographically independent 5,6-dimethylbenzimidazole molecules showing the numbering scheme employed. Non-hydrogen atoms are drawn at the 50% probability level. H atoms are represented by open circles of arbitrary radius. Dashed lines indicate hydrogen bonds.

Table 1. *Fractional atomic coordinates and isotropic thermal parameters with e.s.d.'s*

	x	y	z	B_{iso}*
N(11)	0·17290 (26)	0·12008 (6)	−0·07690 (12)	4·72
N(12)	0·21045 (28)	0·09211 (7)	0·07456 (13)	5·34
N(21)	0·08245 (27)	0·06206 (6)	0·24344 (12)	4·90
N(22)	0·06626 (29)	0·06449 (7)	0·40008 (13)	5·05
N(31)	−0·00165 (27)	0·11095 (6)	0·57006 (12)	4·82
N(32)	0·00708 (27)	0·13358 (6)	0·72321 (12)	4·93
C(11)	0·0942 (3)	0·09319 (9)	−0·01394 (17)	5·30
C(12)	0·3812 (3)	0·12164 (7)	0·06988 (14)	4·20
C(13)	0·35939 (29)	0·13883 (7)	−0·02389 (14)	3·92
C(14)	0·5090 (3)	0·16910 (8)	−0·04949 (15)	4·68
C(15)	0·6803 (3)	0·18232 (8)	0·02186 (18)	4·85
C(16)	0·7016 (3)	0·16556 (8)	0·11810 (18)	5·02
C(17)	0·5542 (4)	0·13497 (8)	0·14147 (15)	5·13
C(18)	0·8444 (4)	0·21522 (10)	−0·00303 (23)	6·95
C(19)	0·8880 (4)	0·18157 (11)	0·19619 (21)	7·26
C(21)	0·1691 (3)	0·07698 (8)	0·33384 (17)	5·15
C(22)	−0·1042 (3)	0·03866 (7)	0·34788 (15)	4·23
C(23)	−0·0977 (3)	0·03704 (7)	0·25050 (14)	4·23
C(24)	−0·2511 (4)	0·01356 (8)	0·18216 (15)	5·11
C(25)	−0·4131 (3)	−0·00891 (8)	0·21454 (19)	5·01
C(26)	−0·4196 (3)	−0·00829 (8)	0·31372 (19)	5·13
C(27)	−0·2668 (4)	0·01559 (8)	0·38016 (16)	5·16
C(28)	−0·5817 (4)	−0·03470 (10)	0·14328 (24)	7·67
C(29)	−0·5884 (4)	−0·03560 (10)	0·34973 (25)	7·28
C(31)	0·0973 (3)	0·10889 (8)	0·66433 (17)	5·12
C(32)	−0·1691 (3)	0·15357 (7)	0·66127 (14)	4·12
C(33)	−0·1769 (3)	0·13978 (7)	0·56628 (14)	4·03
C(34)	−0·3389 (4)	0·15428 (8)	0·49059 (15)	4·90
C(35)	−0·4953 (3)	0·18318 (9)	0·51223 (19)	5·17
C(36)	−0·4892 (3)	0·19726 (8)	0·60885 (20)	5·15
C(37)	−0·3267 (3)	0·18292 (8)	0·68245 (16)	5·01
C(38)	−0·6768 (4)	0·19953 (10)	0·43180 (23)	7·47
C(39)	−0·6610 (4)	0·22871 (10)	0·63107 (25)	7·53

* Calculated from the anisotropic temperature factors of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

Table 2. *Bond distances* (Å), *bond angles* (°) *and hydrogen-bond geometry, with e.s.d.'s in parentheses*

	Molecule 1	Molecule 2	Molecule 3
N(11)–C(11)	1·343 (3)	1·339 (3)	1·342 (3)
N(11)–C(13)	1·381 (2)	1·386 (2)	1·386 (2)
N(12)–C(11)	1·308 (3)	1·307 (3)	1·309 (3)
N(12)–C(12)	1·395 (2)	1·390 (2)	1·395 (2)
C(12)–C(13)	1·380 (3)	1·380 (3)	1·380 (3)
C(12)–C(17)	1·387 (3)	1·396 (3)	1·393 (3)
C(13)–C(14)	1·393 (3)	1·388 (3)	1·385 (3)
C(14)–C(15)	1·377 (3)	1·386 (3)	1·382 (3)
C(15)–C(16)	1·409 (3)	1·404 (3)	1·406 (3)
C(15)–C(18)	1·505 (3)	1·497 (3)	1·516 (3)
C(16)–C(17)	1·375 (3)	1·377 (3)	1·368 (3)
C(16)–C(19)	1·515 (3)	1·512 (3)	1·505 (3)
C(11)–N(11)–C(13)	105·8 (2)	106·0 (2)	106·0 (2)
C(11)–N(12)–C(12)	104·1 (2)	103·6 (2)	103·6 (2)
N(11)–C(11)–N(12)	114·5 (2)	114·7 (2)	114·6 (2)
N(12)–C(12)–C(13)	109·4 (2)	110·3 (2)	110·2 (2)
N(12)–C(12)–C(17)	130·7 (2)	129·9 (2)	130·0 (2)
C(13)–C(12)–C(17)	119·9 (2)	119·8 (2)	119·8 (2)
N(11)–C(13)–C(12)	106·2 (2)	105·4 (2)	105·5 (2)
N(11)–C(13)–C(14)	132·1 (2)	132·7 (2)	132·9 (2)
C(12)–C(13)–C(14)	121·6 (2)	121·9 (2)	121·6 (2)
C(13)–C(14)–C(15)	118·3 (2)	118·0 (2)	118·3 (2)
C(14)–C(15)–C(16)	120·3 (2)	120·7 (2)	120·5 (2)
C(14)–C(15)–C(18)	119·8 (2)	119·7 (2)	120·1 (2)
C(16)–C(15)–C(18)	119·9 (2)	119·6 (2)	119·3 (2)
C(15)–C(16)–C(17)	120·4 (2)	120·4 (2)	120·2 (2)
C(15)–C(16)–C(19)	119·6 (2)	120·5 (2)	119·8 (2)
C(17)–C(16)–C(19)	120·0 (2)	119·0 (2)	120·0 (2)
C(12)–C(17)–C(16)	119·4 (2)	119·2 (2)	119·6 (2)

Intermolecular hydrogen bonds

N—H···N	N···N	H···N	N—H···N
N(11)—H···N(32^{i})	2·807 (2)	1·84	171·2
N(21)—H···N(12)	2·810 (2)	1·81	168·4
N(31)—H···N(22)	2·834 (2)	1·82	174·6

Symmetry code: (i) $x, y, z - 1$.

Peaks corresponding to 33 non-H atoms located in E map and 30 H atoms from subsequent difference Fourier syntheses. Structure refined by full-matrix least-squares; $w(F_o - F_c)$ minimized; $w = 1/\sigma^2(F_o)$ from counting statistics. H positions and thermal parameters refined isotropically by two cycles of least squares with half-shift. Additional refinements were carried to convergence on non-H atoms anisotropically. Final $R = 0{\cdot}045$, $wR = 0{\cdot}060$ for 298 variables, $(\Delta/\sigma)_{\max} = 0{\cdot}01$, maximum positive and negative residual electron density in final difference Fourier map 0·17 and −0·18 e Å^{-3}. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Data reduction carried out using Enraf–Nonius (1983) *SDP* program, a locally modified version of *ALLS* (Lapp & Jacobson, 1979) used for structure refinement, a local modification of *ORFFE* (Busing, Martin & Levy, 1964) for structural parameters with e.s.d.'s. Fig. 1 shows the geometry of three independent molecules and the atomic labelling. Fig. 2 illustrates the molecular packing and hydrogen-bonding scheme. The final atomic coordinates and isotropic thermal parameters are given in Table 1.* Bond lengths and angles in three molecules are given in Table 2.

Related literature. Structures containing the benzimidazole moiety have been reported by Ružić-Toroš (1979), Escande & Galigné (1974), Dik-Edixhoven, Schenk & van der Meer (1973), Trus & Marsh (1973), Sprang & Sundaralingam (1973), and Quick & Williams (1976).

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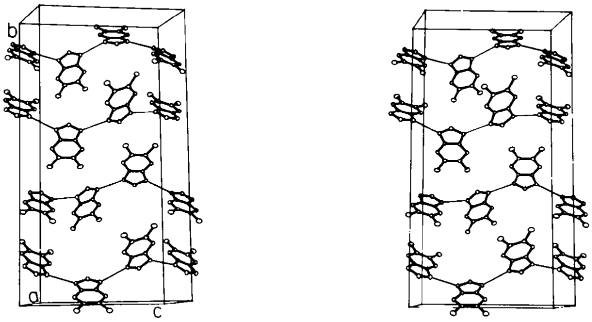

Fig. 2. A view of the packing of molecules in the unit cell. The H atoms are omitted for clarity.

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Structure of (*E*)-2-Butyl-3-triphenylsilyl-2-propenenitrile

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(*Received* 4 *March* 1986; *accepted* 22 *May* 1986)

Abstract. $C_{25}H_{25}NSi$, $M_r = 367{\cdot}6$, triclinic, $P\bar{1}$, $a = 9{\cdot}373\,(1)$, $b = 14{\cdot}690\,(4)$, $c = 9{\cdot}706\,(1)$ Å, $\alpha = 90{\cdot}07\,(1)$, $\beta = 126{\cdot}08\,(2)$, $\gamma = 90{\cdot}88\,(3)°$, $V = 1079{\cdot}9\,(4)$ Å^3, $Z = 2$, $D_x = 1{\cdot}13$, $D_m = 1{\cdot}17\,(3)$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 9{\cdot}9$ cm^{-1}, $F(000) = 392$, ambient temperature, $R = 0{\cdot}055$ for 2704 observations (of 3210 unique data). The molecular structure establishes, unequivocally, that Ni^0-catalysed hydrocyanation of alkynes proceeds in a *syn* fashion [Fitzmaurice, Jackson & Perlmutter (1985).

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