Table 2. *Selected geometric parameters* (Å, °)

O2—C9	1.420 (5)	C1—C15	1.560 (6)
O3—C10	1.423 (5)	C8—C9	1.515 (6)
C1—C2	1.550 (6)	C9—C10	1.552 (5)
C1—C14	1.524 (6)	C10—C11	1.514 (6)
C2—C1—C14	113.3 (4)	C8—C9—C10	111.8 (3)
C2—C1—C15	113.3 (4)	O3—C10—C9	106.9 (3)
C14—C1—C15	110.1 (3)	O3—C10—C11	115.3 (3)
O2—C9—C8	112.1 (3)	C9—C10—C11	109.1 (3)
O2—C9—C10	105.8 (3)		

Data collection: *AFC*-4 (Rigaku Corporation, 1974). Cell refinement: *AFC*-4. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *TEXSAN*. Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *TEXSAN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71701 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1082]

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2,5-Dimethyl-4-nitroimidazole

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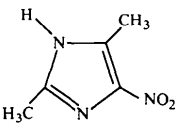
Abstract

The molecules of the title compound, $C_5H_7N_3O_2$, are connected by bifurcated hydrogen bonds and form infinite chains along the **b** direction.

Comment

Nitroimidazoles are known to be either effective radiosensitizers (Farrell, 1989) or antiprotozoic and antibiotic drugs (Edwards, 1981). This investigation of 2,5-dimethyl-4-nitroimidazole (I) is part of an extensive structure-activity study. Perspective views showing the atomic numbering scheme and molecular packing are given in Figs. 1 and 2. The crystal contains



(I)

well ordered molecules of 2,5-dimethyl-4-nitroimidazole in a form also observed in crystals of 4-nitroimidazole (Segalas, Poitras & Beauchamp, 1992; De Bondt, Ragia, Blaton, Peeters & De Ranter, 1993) and 2-methyl-4-nitroimidazole (Kálmán, van Meurs & Toth, 1980). In all these compounds, unsubstituted as well as methyl and dimethyl substituted, the bond lengths and angles of the imidazole ring are in good agreement. The imidazole ring is planar. The maximum deviation from the weighted least-squares plane through non-H atoms is 0.004 (2) Å. As expected, C2—N3 [1.311 (3) Å] shows greater double-bond character than N1—C2 [1.363 (3) Å]. The dihedral angle between the five-membered ring and the nitro group is 177.0 (3)°, and differs from those in the aforementioned structures where the nitro group is coplanar with the ring. This deviation from planarity is caused by hydrogen bonds and molecular crowding in space. The molecules of the title compound, connected by the b_z plane, are linked through bifurcated hydrogen bonds N1—H1···N3^i [2.25 (3) Å, 167 (2)°] and N1—H1···O401^i [2.57 (3) Å, 121 (2)°; symmetry code: (i) x, $\frac{1}{2}+y$, $\frac{1}{2}-z$] and form infinite chains along the **b** direction. In comparison to 4-nitroimidazole and 2-methyl-4-nitroimidazole, the weighted least-squares planes through the neighbouring imidazoles cross at an angle of 133.5 (1)° instead of being coplanar. This deviation from coplanarity is probably caused by steric hindrance due to the 2,5-dimethyl substituents.

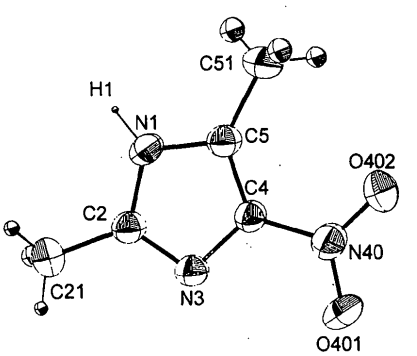


Fig. 1. A perspective view of the molecule with atomic numbering scheme. The displacement ellipsoids are plotted at the 50% probability level.

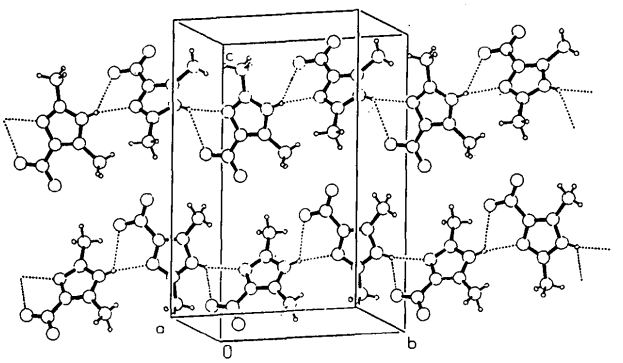


Fig. 2. Chains of molecules linked by hydrogen bonds along the *b* axis.

Experimental

Crystal data

$C_5H_7N_3O_2$
M_r = 141.13
Orthorhombic
Pcab
a = 7.724 (1) Å
b = 10.513 (1) Å
c = 16.034 (3) Å
V = 1302.0 (3) Å^3
Z = 8
D_x = 1.440 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 22 reflections
θ = 10.08-13.97°
μ = 0.1068 mm^{-1}
T = 293 K
Needle
0.15 × 0.10 × 0.10 mm
Colourless

Data collection

Stoe Stadi-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2650 measured reflections
1103 independent reflections
735 observed reflections [$I > 2.0\sigma(I)$]
R_{int} = 0.014
θ_{max} = 25.0°
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 13$
$l = -19 \rightarrow 19$
3 standard reflections
frequency: 60 min
intensity variation: < 3.0%

Refinement

Refinement on F
R = 0.0377
wR = 0.0349
S = 0.7693
735 reflections
119 parameters
All H-atom parameters refined
Unit weights applied
$(\Delta/\sigma)_{max}$ = 0.018
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *CRYSRULER* (Rizzoli, Sangermano, Calestani & Andreetti, 1989)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1	0.0640 (3)	0.8586 (2)	0.2653 (1)	0.0379 (9)
C2	0.0261 (3)	0.7496 (3)	0.2231 (1)	0.0356 (7)
C21	−0.0471 (5)	0.7488 (4)	0.1372 (2)	0.0476 (9)
N3	0.0638 (3)	0.6487 (2)	0.2676 (1)	0.0361 (8)
C4	0.1298 (4)	0.6985 (2)	0.3403 (2)	0.0340 (9)
N40	0.1885 (4)	0.6167 (2)	0.4045 (2)	0.0447 (9)
O401	0.1749 (4)	0.5016 (2)	0.3947 (1)	0.073 (1)
O402	0.2541 (4)	0.6643 (2)	0.4672 (1)	0.067 (8)
C5	0.1321 (4)	0.8280 (2)	0.3409 (2)	0.036 (1)
C51	0.1864 (6)	0.9251 (3)	0.4030 (2)	0.054 (1)

Table 2. *Selected geometric parameters* (Å, °)

N1—C2	1.363 (3)	C4—N40	1.416 (4)
N1—C5	1.360 (3)	C4—C5	1.362 (3)
N1—H1	0.86 (2)	N40—O401	1.225 (3)
C2—C21	1.489 (3)	N40—O402	1.232 (3)
C2—N3	1.311 (3)	C5—C51	1.486 (4)
N3—C4	1.376 (3)		
C5—N1—H1	122 (2)	N3—C4—N40	120.2 (2)
C2—N1—H1	128 (2)	N40—C4—C5	126.7 (3)
C2—N1—C5	109.1 (2)	C4—N40—O402	118.6 (2)
N1—C2—N3	111.3 (2)	C4—N40—O401	118.6 (3)
N1—C2—C21	123.1 (3)	O401—N40—O402	122.8 (2)
C21—C2—N3	125.7 (2)	N1—C5—C4	103.0 (3)
C2—N3—C4	103.6 (2)	C4—C5—C51	134.0 (3)
N3—C4—C5	113.0 (3)	N1—C5—C51	122.9 (2)

Data collection: *DIF4* (Stoe & Cie, 1992*a*). Cell refinement: *DIF4*. Data reduction: *REDU4* (Stoe & Cie, 1992*b*). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELX76* (Sheldrick, 1976). Molecular graphics: *ORTEP*II (Johnson, 1976); *PLUTON93* (Spek, 1993). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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