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2-(1-Benzyl-5-methyl-1*H*-imidazol-4-yl)-1,3,4-oxadiazole

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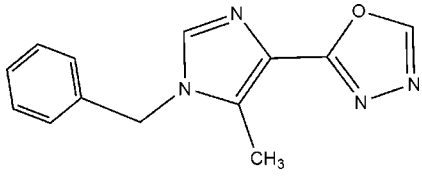
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.147; data-to-parameter ratio = 9.3.

In the title imidazole derivative, $C_{13}H_{12}N_4O$, the two heterocyclic rings are almost coplanar [dihedral angle = 0.9 (2)°]. The phenyl ring, however, is almost perpendicular to the central ring [dihedral angle = 75.8 (2)°]. The crystal packing is consolidated by weak C—H···N interactions.

Related literature

For related literature, see: Chen *et al.* (2005); Teng *et al.* (2005); Benkli (2004); Frank (2006).



Experimental

Crystal data

$C_{13}H_{12}N_4O$
M_r = 240.27
Monoclinic, $P2_1$
a = 4.5880 (1) Å
b = 8.1255 (2) Å
c = 16.1240 (8) Å
β = 93.074 (1)°
V = 600.23 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.20 × 0.10 × 0.02 mm

Data collection

Bruker SMART 4 K CCD area detector diffractometer
Absorption correction: none
5797 measured reflections
1518 independent reflections
1143 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.147
S = 1.10
1518 reflections
164 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11*C*···N3	0.96	2.57	3.226 (6)	126
C13—H13···N2^{i}	0.93	2.39	3.302 (5)	165
C7—H7*A*···N4^{ii}	0.97	2.61	3.533 (5)	158

Symmetry codes: (i) $-x+3, y-\frac{1}{2}, -z+1$; (ii) $x-1, y+1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2413).

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supplementary materials

Acta Cryst. (2007). E**63**, o2976 [**doi:10.1107/S1600536807023483**]

2-(1-Benzyl-5-methyl-1*H*-imidazol-4-yl)-1,3,4-oxadiazole

J. Li

Comment

Imidazole derivatives have many biological properties, such as antibacterial and antifungal activities (Frank *et al.*, 2006; Benkli, 2004). Our group has synthesized a novel class of 2-(1-benzyl-4-methyl-1*H*-imidazol-4-yl)-1,3,4-oxadiazole analogues. In this paper, we present the structure of one such analogue, the title compound (I).

Rings A (O1/N3–4/C12–13) and ring B (N1–2/C8—C10) are almost coplanar with a dihedral angle of 0.9 (2)°. The dihedral angle between the central ring and the terminal aromatic ring (C1—C6) is 75.8 (2)°. The weak C—H···N intramolecular and intermolecular hydrogen bonds (Table 1) give rise to a three dimensional network (Fig. 2).

Experimental

2-(4-methyl-1*H*-imidazol-4-yl)-1,3,4-oxadiazole (0.18 g, 1.2 mmol) was dissolved in DMF (2 ml), then 60% sodium hydride (58 mg, 1.44 mmol), was added, and after stirring for 30 minutes at room temperature, benzyl bromide (0.31 g, 1.8 mmol) was added dropwise. The reaction mixture was poured into water until the consumption of the starting material, as monitored by TLC. Then, the product was extracted with ethyl acetate, whcih was dried and concentrated. The reside was chromatographed (acetone/petroleum ether, 1:5 *v*/*v*). The yield of the title compound is 43%. Colourless plates of (I) were grown from an acetone solution at 288 K (r.t.).^{1}H NMR (CDCl3, 400 MHz): σ 8.43 (s, 1 H), 7.68 (s, 1 H), 7.39 − 7.11 (m, 5 H), 5.18 (s, 2 H), 2.57 (s, 3 H).

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

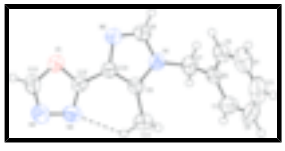

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level (arbitrary spheres for the H atoms).

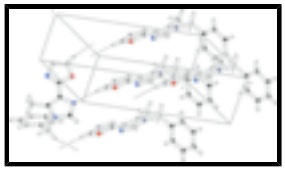

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

2-(1-benzyl-5-methyl-1*H*-imidazol-4-yl)-1,3,4-oxadiazole

Crystal data

$C_{13}H_{12}N_4O$	$F_{000} = 252$
$M_r = 240.27$	$D_x = 1.329$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1201 reflections
$a = 4.5880$ (1) Å	$\theta = 2.5$–20.4º
$b = 8.1255$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 16.1240$ (8) Å	$T = 295$ (2) K
$\beta = 93.074$ (1)º	Plate, colorless
$V = 600.23$ (4) Å^3	0.20 × 0.10 × 0.02 mm
$Z = 2$	

Data collection

Bruker SMART 4K CCD area detector diffractometer	1143 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.037$
Monochromator: graphite	$\theta_{max} = 28.0$º
$T = 295$(2) K	$\theta_{min} = 1.3$º
ω scans	$h = -6 \rightarrow 6$
Absorption correction: none	$k = -10 \rightarrow 10$
5797 measured reflections	$l = -20 \rightarrow 21$
1518 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.0821P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = <0.001$
1518 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5507 (9)	0.3950 (6)	0.0930 (2)	0.0671 (11)
H1	0.4139	0.3110	0.0860	0.081*
C2	0.6742 (13)	0.4632 (8)	0.0241 (2)	0.0899 (17)
H2	0.6190	0.4262	−0.0290	0.108*
C3	0.8794 (11)	0.5866 (8)	0.0352 (3)	0.0865 (16)
H3	0.9645	0.6323	−0.0106	0.104*
C4	0.9576 (10)	0.6415 (6)	0.1133 (3)	0.0809 (14)
H4	1.0963	0.7245	0.1206	0.097*
C5	0.8343 (8)	0.5759 (5)	0.1802 (2)	0.0596 (10)
H5	0.8879	0.6155	0.2329	0.072*
C6	0.6298 (7)	0.4511 (4)	0.17146 (19)	0.0460 (7)
C7	0.4958 (7)	0.3825 (5)	0.2474 (2)	0.0544 (9)
H7A	0.4159	0.4722	0.2787	0.065*
H7B	0.3362	0.3098	0.2301	0.065*
C8	0.8387 (8)	0.3479 (5)	0.3730 (2)	0.0570 (9)
H8	0.8008	0.4508	0.3952	0.068*
C9	0.8167 (7)	0.1368 (4)	0.28808 (19)	0.0452 (7)
C10	1.0097 (7)	0.1096 (4)	0.35461 (19)	0.0450 (7)
C11	0.7285 (10)	0.0334 (5)	0.2150 (2)	0.0672 (11)
H11A	0.8162	0.0757	0.1667	0.101*
H11B	0.5199	0.0353	0.2063	0.101*
H11C	0.7925	−0.0778	0.2248	0.101*
C12	1.1856 (7)	−0.0360 (4)	0.37196 (17)	0.0460 (7)
C13	1.4927 (9)	−0.1875 (5)	0.4375 (2)	0.0623 (10)
H13	1.6279	−0.2270	0.4777	0.075*
N4	1.4110 (8)	−0.2676 (4)	0.3739 (2)	0.0716 (10)
N1	0.7076 (6)	0.2910 (4)	0.30149 (15)	0.0474 (7)
N2	1.0229 (7)	0.2439 (4)	0.40749 (16)	0.0547 (8)
O1	1.3644 (5)	−0.0374 (3)	0.44171 (13)	0.0549 (7)
N3	1.2055 (7)	−0.1670 (4)	0.3294 (2)	0.0680 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.078 (2)	0.060 (2)	0.062 (2)	0.012 (2)	−0.013 (2)	−0.0128 (19)
C2	0.118 (4)	0.109 (4)	0.0416 (19)	0.057 (4)	−0.001 (2)	0.002 (2)
C3	0.089 (3)	0.094 (4)	0.079 (3)	0.035 (3)	0.025 (3)	0.035 (3)
C4	0.077 (3)	0.066 (3)	0.101 (4)	0.003 (2)	0.013 (2)	0.026 (3)
C5	0.065 (2)	0.048 (2)	0.065 (2)	0.0077 (19)	−0.0021 (18)	0.0040 (18)
C6	0.0452 (17)	0.0394 (16)	0.0530 (17)	0.0101 (15)	−0.0011 (13)	0.0027 (15)
C7	0.0487 (17)	0.053 (2)	0.0606 (19)	0.0103 (17)	−0.0013 (16)	0.0051 (18)
C8	0.078 (2)	0.0463 (19)	0.0473 (17)	0.0119 (18)	0.0054 (17)	−0.0060 (15)
C9	0.0501 (17)	0.0390 (17)	0.0466 (17)	−0.0021 (15)	0.0040 (14)	0.0018 (14)
C10	0.0547 (18)	0.0402 (17)	0.0403 (15)	−0.0029 (15)	0.0031 (14)	0.0006 (13)
C11	0.086 (3)	0.054 (2)	0.060 (2)	0.001 (2)	−0.0166 (19)	−0.0090 (18)
C12	0.0536 (19)	0.0443 (17)	0.0399 (15)	−0.0010 (15)	0.0008 (13)	−0.0009 (15)
C13	0.074 (2)	0.054 (2)	0.058 (2)	0.017 (2)	−0.0033 (18)	0.0089 (18)
N4	0.089 (3)	0.0551 (19)	0.069 (2)	0.0212 (18)	−0.0092 (18)	−0.0049 (17)
N1	0.0526 (15)	0.0486 (15)	0.0411 (13)	0.0041 (13)	0.0039 (11)	0.0025 (12)
N2	0.072 (2)	0.0455 (18)	0.0456 (15)	0.0060 (15)	−0.0034 (13)	−0.0047 (13)
O1	0.0716 (16)	0.0500 (13)	0.0419 (11)	0.0056 (13)	−0.0074 (10)	0.0031 (11)
N3	0.081 (2)	0.055 (2)	0.0664 (19)	0.0147 (18)	−0.0152 (17)	−0.0173 (16)

Geometric parameters (Å, °)

C1—C6	1.376 (5)	C8—N1	1.353 (4)
C1—C2	1.388 (7)	C8—H8	0.9300
C1—H1	0.9300	C9—N1	1.371 (4)
C2—C3	1.380 (8)	C9—C10	1.372 (5)
C2—H2	0.9300	C9—C11	1.485 (5)
C3—C4	1.366 (7)	C10—N2	1.384 (4)
C3—H3	0.9300	C10—C12	1.452 (5)
C4—C5	1.353 (6)	C11—H11A	0.9600
C4—H4	0.9300	C11—H11B	0.9600
C5—C6	1.384 (5)	C11—H11C	0.9600
C5—H5	0.9300	C12—N3	1.272 (5)
C6—C7	1.506 (5)	C12—O1	1.356 (4)
C7—N1	1.472 (4)	C13—N4	1.254 (5)
C7—H7A	0.9700	C13—O1	1.357 (5)
C7—H7B	0.9700	C13—H13	0.9300
C8—N2	1.299 (5)	N4—N3	1.414 (4)
C6—C1—C2	120.3 (5)	N1—C8—H8	123.5
C6—C1—H1	119.9	N1—C9—C10	104.4 (3)
C2—C1—H1	119.9	N1—C9—C11	123.8 (3)
C3—C2—C1	119.4 (4)	C10—C9—C11	131.8 (3)
C3—C2—H2	120.3	C9—C10—N2	111.1 (3)
C1—C2—H2	120.3	C9—C10—C12	127.6 (3)
C4—C3—C2	120.0 (4)	N2—C10—C12	121.2 (3)

C4—C3—H3	120.0	C9—C11—H11A	109.5
C2—C3—H3	120.0	C9—C11—H11B	109.5
C5—C4—C3	120.4 (4)	H11A—C11—H11B	109.5
C5—C4—H4	119.8	C9—C11—H11C	109.5
C3—C4—H4	119.8	H11A—C11—H11C	109.5
C4—C5—C6	121.2 (4)	H11B—C11—H11C	109.5
C4—C5—H5	119.4	N3—C12—O1	112.5 (3)
C6—C5—H5	119.4	N3—C12—C10	129.3 (3)
C1—C6—C5	118.7 (4)	O1—C12—C10	118.2 (3)
C1—C6—C7	121.8 (4)	N4—C13—O1	113.3 (3)
C5—C6—C7	119.5 (3)	N4—C13—H13	123.3
N1—C7—C6	112.5 (3)	O1—C13—H13	123.3
N1—C7—H7A	109.1	C13—N4—N3	106.1 (3)
C6—C7—H7A	109.1	C8—N1—C9	107.3 (3)
N1—C7—H7B	109.1	C8—N1—C7	125.6 (3)
C6—C7—H7B	109.1	C9—N1—C7	127.1 (3)
H7A—C7—H7B	107.8	C8—N2—C10	104.1 (3)
N2—C8—N1	113.1 (3)	C12—O1—C13	102.1 (3)
N2—C8—H8	123.5	C12—N3—N4	105.9 (3)
C6—C1—C2—C3	0.7 (7)	O1—C13—N4—N3	−0.5 (5)
C1—C2—C3—C4	−0.6 (7)	N2—C8—N1—C9	−0.2 (4)
C2—C3—C4—C5	−0.2 (7)	N2—C8—N1—C7	−178.1 (3)
C3—C4—C5—C6	0.8 (6)	C10—C9—N1—C8	0.5 (3)
C2—C1—C6—C5	−0.1 (6)	C11—C9—N1—C8	−179.4 (3)
C2—C1—C6—C7	178.7 (4)	C10—C9—N1—C7	178.4 (3)
C4—C5—C6—C1	−0.6 (5)	C11—C9—N1—C7	−1.5 (5)
C4—C5—C6—C7	−179.5 (3)	C6—C7—N1—C8	102.4 (4)
C1—C6—C7—N1	113.2 (4)	C6—C7—N1—C9	−75.1 (4)
C5—C6—C7—N1	−68.0 (4)	N1—C8—N2—C10	−0.2 (4)
N1—C9—C10—N2	−0.7 (4)	C9—C10—N2—C8	0.5 (4)
C11—C9—C10—N2	179.3 (4)	C12—C10—N2—C8	−179.6 (3)
N1—C9—C10—C12	179.5 (3)	N3—C12—O1—C13	−1.2 (4)
C11—C9—C10—C12	−0.5 (6)	C10—C12—O1—C13	−179.5 (3)
C9—C10—C12—N3	1.8 (6)	N4—C13—O1—C12	1.0 (4)
N2—C10—C12—N3	−178.0 (4)	O1—C12—N3—N4	0.9 (4)
C9—C10—C12—O1	179.8 (3)	C10—C12—N3—N4	179.0 (3)
N2—C10—C12—O1	0.0 (5)	C13—N4—N3—C12	−0.3 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11C···N3	0.96	2.57	3.226 (6)	126
C13—H13···N2^{i}	0.93	2.39	3.302 (5)	165
C7—H7A···N4^{ii}	0.97	2.61	3.533 (5)	158

Symmetry codes: (i) −*x*+3, *y*−1/2, −*z*+1; (ii) *x*−1, *y*+1, *z*.

Fig. 1

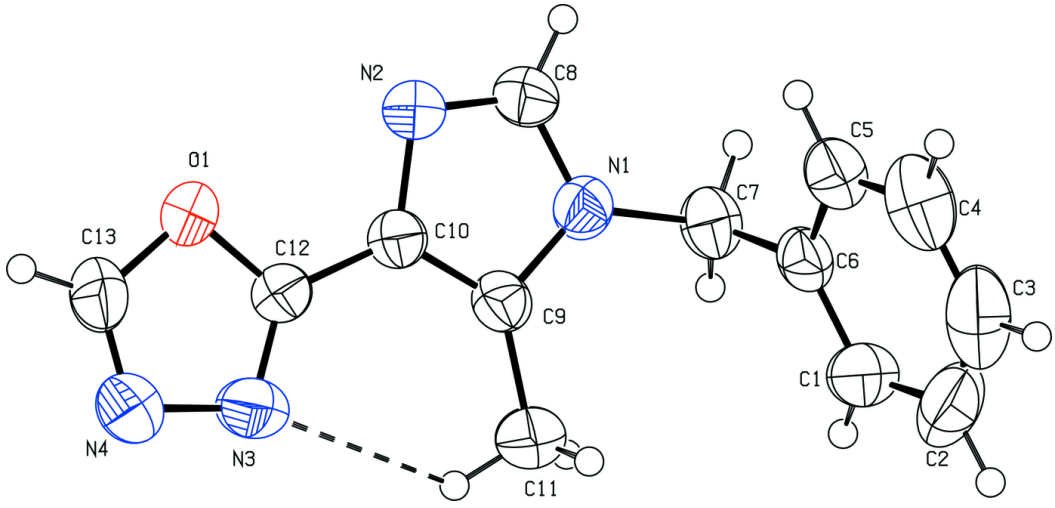

Fig. 2