Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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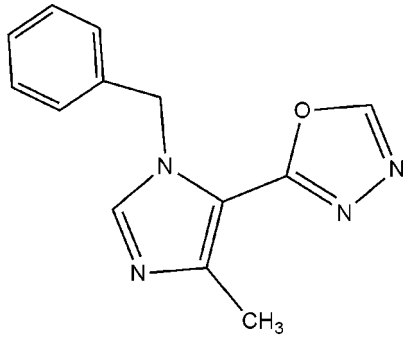
Received 16 May 2007; accepted 16 May 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 15.5.

In the title compound, $C_{13}H_{12}N_4O$, the C_2N_2O and C_3N_2 heterocyclic rings are almost coplanar, with a dihedral angle of 9.17 (10)°. The dihedral angle between the C_3N_2 ring and the pendant phenyl ring is 88.69 (9)°. In the crystal structure, weak C—H···N hydrogen bonds link the molecules into a chain propagating along the b axis. Further stability is provided by offset π–π stacking interactions of 3.48 (1)–3.83 (1) Å. Further stability is provided by offset π–π stacking interactions of 3.48 (1)–3.83 (1) Å (centroid-to-centroid) involving the imidazole and oxadiazole rings.

Related literature

For background literature, see: Frank (2006); Benkli (2004). For related literature, see: Allen *et al.* (1987); Janiak (2000).



Experimental

Crystal data

$C_{13}H_{12}N_4O$
M_r = 240.27
Monoclinic, $P2_1/n$
a = 10.9098 (12) Å
b = 8.7854 (10) Å
c = 13.0367 (14) Å
β = 111.031 (2)°
V = 1166.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: none
8407 measured reflections
2541 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.06
2541 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···N2^{i}	0.93	2.47	3.227 (2)	139
C8—H8···N4^{ii}	0.93	2.49	3.233 (2)	137

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

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).

The authors thank Dr Wei Huang for technical assistance and Dr Xiang-Gao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2417).

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supplementary materials

Acta Cryst. (2007). E**63**, o2977 [**doi:10.1107/S1600536807024129**]

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

J. Li and H.-B. Zhou

Comment

Imidazole derivatives have many biological properties, such as antibacterial and antifungal activities (Frank, 2006; Benkli, 2004). Our group synthesized a novel class of 2-(1-benzyl-4-methyl-1*H*-imidazol-5-yl)-1,3,4-oxadiazole analogues. In this paper, we present the structure of one such analogue, the title compound (I).

Ring A (O1/N3–4/C12–13) and ring B (N1–2/C8—C10) are nearlly coplanar with a dihedral angle of 9.17 (10)°. The dihedral angle between ring B and C (C1—C6) is 88.69 (3)°.

In the crystal structure C—H···N hydrogen bonds link the molecules into rows along the *b* axis (Table 1). Further stability is provided by offset π-π stacking interactions (Janiak, 2000) involving rings A and B. The distance between the adjacent ring centroids for A···A is 3.48 (1)Å (symmetry code linking the adjacent rings: $1 - x, -y, -z$). The distance between the adjacent ring centroids of ring B is 3.56 (1)Å (symmetry code linking the adjacent rings: $1 - x, 1 - y, -z$). A further interaction occurs between adjacent A and B rings (symmetry codes $3/2 - x,-1/2 + y,1/2 - z$; $3/2 - x,1/2 + y,1/2 - z$) with a centroid to centroid distance of 3.83 (1) Å, Figure 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), and then added 60% sodium hydride (58 mg, 1.44 mmol) was added. 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 after the consumption of the starting material (monitored by TLC tracing). Then, it was extracted with ethyl acetate. The ethyl acetate phase was dried and concentrated. The reside was chromatographed (acetone/petroleum ether, 1:5 *v*/*v*) The yield of compound (I) is 17%. Colourless slabs of (I) suitable for X-ray diffraction were grown from an acetone solution at 288 K

^{1}H NMR (CDCl3, 400 MHz): σ 8.42 (s, 1 H), 7.64 (s, 1 H), 7.33–7.21 (m, 5 H), 5.65 (s, 2 H), 2.57 (s, 3 H)

Refinement

All H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

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

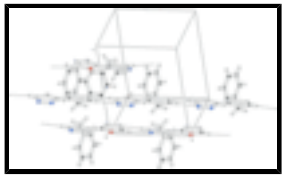

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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

Crystal data

$C_{13}H_{12}N_4O$	F_{000} = 504
M_r = 240.27	D_x = 1.368 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3057 reflections
a = 10.9098 (12) Å	θ = 2.9–27.0º
b = 8.7854 (10) Å	μ = 0.09 mm^{-1}
c = 13.0367 (14) Å	T = 297 (2) K
β = 111.031 (2)º	Slab, colourless
V = 1166.3 (2) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2139 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.029
Monochromator: graphite	θ_{max} = 27.0º
T = 297(2) K	θ_{min} = 2.1º
ω scans	h = −13→13
Absorption correction: none	k = −11→11
8407 measured reflections	l = −16→16
2541 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

$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2 + 0.2589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2541 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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	1.00271 (17)	0.40873 (19)	0.16228 (14)	0.0443 (4)
H1	0.9675	0.4882	0.1899	0.053*
C2	1.12452 (18)	0.3507 (2)	0.22466 (16)	0.0547 (5)
H2	1.1699	0.3897	0.2944	0.066*
C3	1.17854 (19)	0.2351 (2)	0.18338 (18)	0.0572 (5)
H3	1.2605	0.1960	0.2252	0.069*
C4	1.1117 (2)	0.1776 (2)	0.08079 (18)	0.0568 (5)
H4	1.1489	0.1005	0.0526	0.068*
C5	0.98848 (18)	0.23419 (18)	0.01881 (16)	0.0486 (4)
H5	0.9431	0.1940	−0.0505	0.058*
C6	0.93259 (15)	0.35029 (17)	0.05944 (13)	0.0370 (4)
C7	0.79990 (16)	0.41293 (18)	−0.00980 (13)	0.0408 (4)
H7A	0.8123	0.5036	−0.0474	0.049*
H7B	0.7545	0.3384	−0.0653	0.049*
C8	0.69045 (17)	0.59261 (17)	0.07816 (15)	0.0449 (4)
H8	0.7197	0.6798	0.0536	0.054*
C9	0.59728 (15)	0.44629 (18)	0.15841 (13)	0.0388 (4)
C10	0.65791 (13)	0.35388 (17)	0.10545 (12)	0.0340 (3)
C11	0.51846 (19)	0.4036 (2)	0.22652 (17)	0.0556 (5)
H11A	0.4870	0.4941	0.2502	0.083*
H11B	0.5724	0.3471	0.2896	0.083*
H11C	0.4452	0.3422	0.1837	0.083*
C12	0.65801 (13)	0.19092 (17)	0.09258 (12)	0.0338 (3)
C13	0.62176 (17)	−0.03845 (17)	0.11956 (14)	0.0440 (4)

H13	0.5958	−0.1256	0.1468	0.053*
N1	0.71746 (12)	0.45100 (13)	0.05361 (11)	0.0369 (3)
N2	0.61863 (14)	0.59569 (15)	0.14023 (12)	0.0468 (4)
N3	0.69886 (14)	0.11157 (15)	0.02825 (12)	0.0452 (4)
N4	0.67448 (14)	−0.04186 (15)	0.04746 (13)	0.0471 (4)
O1	0.60662 (11)	0.10365 (12)	0.15336 (9)	0.0414 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0522 (10)	0.0421 (9)	0.0453 (9)	0.0004 (7)	0.0256 (8)	0.0001 (7)
C2	0.0538 (11)	0.0572 (11)	0.0516 (10)	−0.0056 (8)	0.0171 (9)	0.0064 (8)
C3	0.0465 (10)	0.0536 (11)	0.0754 (14)	0.0044 (8)	0.0268 (10)	0.0193 (10)
C4	0.0610 (11)	0.0406 (9)	0.0852 (14)	0.0075 (8)	0.0462 (11)	0.0051 (9)
C5	0.0588 (11)	0.0396 (9)	0.0579 (11)	−0.0029 (8)	0.0338 (9)	−0.0055 (8)
C6	0.0457 (8)	0.0305 (7)	0.0438 (9)	−0.0037 (6)	0.0268 (7)	0.0029 (6)
C7	0.0501 (9)	0.0377 (8)	0.0406 (8)	−0.0013 (7)	0.0237 (7)	0.0047 (6)
C8	0.0497 (9)	0.0268 (8)	0.0593 (10)	0.0016 (6)	0.0209 (8)	0.0032 (7)
C9	0.0362 (8)	0.0346 (8)	0.0455 (9)	0.0021 (6)	0.0148 (7)	−0.0019 (6)
C10	0.0343 (7)	0.0286 (7)	0.0398 (8)	−0.0009 (5)	0.0141 (6)	0.0010 (6)
C11	0.0542 (11)	0.0572 (11)	0.0679 (12)	0.0044 (8)	0.0370 (10)	−0.0022 (9)
C12	0.0338 (7)	0.0297 (7)	0.0394 (8)	−0.0008 (5)	0.0148 (6)	0.0022 (6)
C13	0.0519 (9)	0.0270 (7)	0.0550 (10)	−0.0021 (7)	0.0215 (8)	0.0023 (7)
N1	0.0412 (7)	0.0274 (6)	0.0449 (7)	−0.0001 (5)	0.0188 (6)	0.0030 (5)
N2	0.0502 (8)	0.0334 (7)	0.0592 (9)	0.0054 (6)	0.0224 (7)	−0.0021 (6)
N3	0.0559 (8)	0.0305 (7)	0.0585 (9)	−0.0021 (6)	0.0318 (7)	−0.0024 (6)
N4	0.0557 (9)	0.0285 (7)	0.0634 (9)	0.0004 (6)	0.0290 (7)	−0.0013 (6)
O1	0.0522 (7)	0.0304 (5)	0.0477 (7)	−0.0037 (5)	0.0252 (5)	0.0011 (5)

Geometric parameters (Å, °)

C1—C6	1.382 (2)	C8—N1	1.3435 (19)
C1—C2	1.383 (3)	C8—H8	0.9300
C1—H1	0.9300	C9—N2	1.369 (2)
C2—C3	1.377 (3)	C9—C10	1.379 (2)
C2—H2	0.9300	C9—C11	1.489 (2)
C3—C4	1.369 (3)	C10—N1	1.3863 (18)
C3—H3	0.9300	C10—C12	1.441 (2)
C4—C5	1.388 (3)	C11—H11A	0.9600
C4—H4	0.9300	C11—H11B	0.9600
C5—C6	1.387 (2)	C11—H11C	0.9600
C5—H5	0.9300	C12—N3	1.2870 (19)
C6—C7	1.508 (2)	C12—O1	1.3597 (17)
C7—N1	1.4621 (19)	C13—N4	1.266 (2)
C7—H7A	0.9700	C13—O1	1.3536 (19)
C7—H7B	0.9700	C13—H13	0.9300
C8—N2	1.313 (2)	N3—N4	1.4137 (18)
C6—C1—C2	120.94 (16)	N1—C8—H8	123.3

C6—C1—H1	119.5	N2—C9—C10	109.63 (13)
C2—C1—H1	119.5	N2—C9—C11	121.02 (14)
C3—C2—C1	119.86 (19)	C10—C9—C11	129.35 (15)
C3—C2—H2	120.1	C9—C10—N1	105.94 (13)
C1—C2—H2	120.1	C9—C10—C12	131.58 (13)
C4—C3—C2	120.07 (18)	N1—C10—C12	122.30 (12)
C4—C3—H3	120.0	C9—C11—H11A	109.5
C2—C3—H3	120.0	C9—C11—H11B	109.5
C3—C4—C5	120.08 (17)	H11A—C11—H11B	109.5
C3—C4—H4	120.0	C9—C11—H11C	109.5
C5—C4—H4	120.0	H11A—C11—H11C	109.5
C6—C5—C4	120.50 (18)	H11B—C11—H11C	109.5
C6—C5—H5	119.7	N3—C12—O1	112.70 (13)
C4—C5—H5	119.7	N3—C12—C10	128.96 (13)
C1—C6—C5	118.51 (16)	O1—C12—C10	118.32 (12)
C1—C6—C7	121.55 (14)	N4—C13—O1	113.86 (14)
C5—C6—C7	119.91 (15)	N4—C13—H13	123.1
N1—C7—C6	113.46 (12)	O1—C13—H13	123.1
N1—C7—H7A	108.9	C8—N1—C10	105.82 (13)
C6—C7—H7A	108.9	C8—N1—C7	125.35 (13)
N1—C7—H7B	108.9	C10—N1—C7	128.74 (12)
C6—C7—H7B	108.9	C8—N2—C9	105.26 (13)
H7A—C7—H7B	107.7	C12—N3—N4	105.65 (13)
N2—C8—N1	113.34 (14)	C13—N4—N3	105.87 (12)
N2—C8—H8	123.3	C13—O1—C12	101.91 (12)
C6—C1—C2—C3	1.3 (3)	N2—C8—N1—C10	−0.4 (2)
C1—C2—C3—C4	−0.1 (3)	N2—C8—N1—C7	−177.16 (15)
C2—C3—C4—C5	−1.0 (3)	C9—C10—N1—C8	0.27 (16)
C3—C4—C5—C6	0.7 (3)	C12—C10—N1—C8	175.98 (14)
C2—C1—C6—C5	−1.5 (2)	C9—C10—N1—C7	176.91 (15)
C2—C1—C6—C7	−179.69 (14)	C12—C10—N1—C7	−7.4 (2)
C4—C5—C6—C1	0.5 (2)	C6—C7—N1—C8	106.34 (18)
C4—C5—C6—C7	178.70 (14)	C6—C7—N1—C10	−69.7 (2)
C1—C6—C7—N1	−39.5 (2)	N1—C8—N2—C9	0.3 (2)
C5—C6—C7—N1	142.33 (14)	C10—C9—N2—C8	−0.13 (19)
N2—C9—C10—N1	−0.09 (17)	C11—C9—N2—C8	179.98 (16)
C11—C9—C10—N1	179.79 (17)	O1—C12—N3—N4	−0.57 (18)
N2—C9—C10—C12	−175.24 (15)	C10—C12—N3—N4	−179.21 (14)
C11—C9—C10—C12	4.6 (3)	O1—C13—N4—N3	−0.1 (2)
C9—C10—C12—N3	167.80 (17)	C12—N3—N4—C13	0.38 (19)
N1—C10—C12—N3	−6.7 (2)	N4—C13—O1—C12	−0.26 (19)
C9—C10—C12—O1	−10.8 (2)	N3—C12—O1—C13	0.53 (17)
N1—C10—C12—O1	174.76 (13)	C10—C12—O1—C13	179.32 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···N2^{i}	0.93	2.47	3.227 (2)	139

C8—H8···N4^{ii}	0.93	2.49	3.233 (2)	137

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

Fig. 1

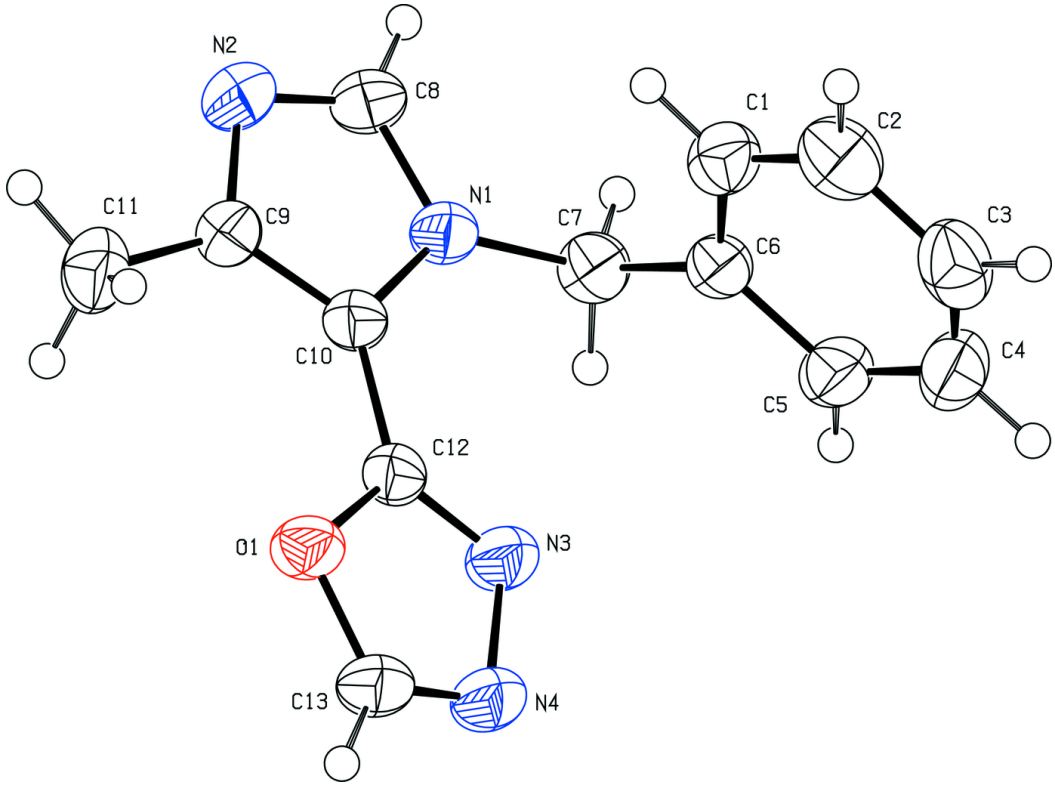

Fig. 2