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2-(3-Benzyloxy-4-methoxyphenyl)-5-phenyl-1,3,4-oxadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.035
wR factor = 0.104
Data-to-parameter ratio = 11.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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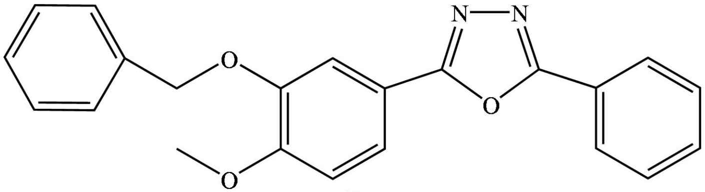
The title compound, $C_{22}H_{18}N_2O_3$, was synthesized by oxidation of benzoic acid (3-benzyloxy-4-methoxybenzylidene)hydrazide with bis(trifluoroacetoxy)iodobenzene in chloroform at room temperature.

Comment

Symmetrical and unsymmetrical 1,3,4-oxadiazoles have been reported to be versatile compounds displaying a variety of biological effects, which include anti-inflammatory (Omar *et al.*, 1996), antifungal (Talawar *et al.*, 1996) and antimicrobial (Hamad *et al.*, 1996) activities. They have been utilized as bioisosteres of the carboxamide moiety in benzodiazepine receptor agonists, muscarinic receptor agonists, NK1 receptor antagonists, and Phe–Gly peptidomimetics (Tully *et al.*, 1991; Barry *et al.*, 1991; Ladduwahetty *et al.*, 1996; Borg *et al.*, 1999). Moreover, oxadiazole derivatives have been widely used as electron-conducting and hole-blocking materials in molecule-based as well as polymeric light-emitting devices (LEDs) due to the electron-deficient and favourable electron-transport properties of the oxadiazole rings (Brown *et al.*, 1992).



(I)

The title compound, (I), was synthesized by oxidation of benzoic acid (3-benzyloxy-4-methoxybenzylidene)hydrazide with bis(trifluoroacetoxy)iodobenzene in chloroform at room temperature.

The molecular structure of (I) is illustrated in Fig. 1. Bond distances and angles are as expected (Table 1). The C3–C8 and C9–C14 benzene rings are nearly coplanar with the oxadiazole ring, the dihedral angles they form with it being 6.27 (4) and 5.96 (4)°, respectively. The crystal packing is stabilized mainly by van der Waals interactions.

Experimental

A dry round-bottomed flask was charged with benzoic acid (3-benzyloxy-4-methoxybenzylidene)hydrazide (1 mmol), bis(trifluoroacetoxy)iodobenzene (1.2 mmol) and chloroform (5 ml). This mixture was stirred at room temperature and monitored by thin-layer chromatography. When the reaction was complete, the product was purified directly by flash chromatography (silica gel, ethyl acetate/petroleum ether 3:1) to afford the product as a white solid (m.p. 447–

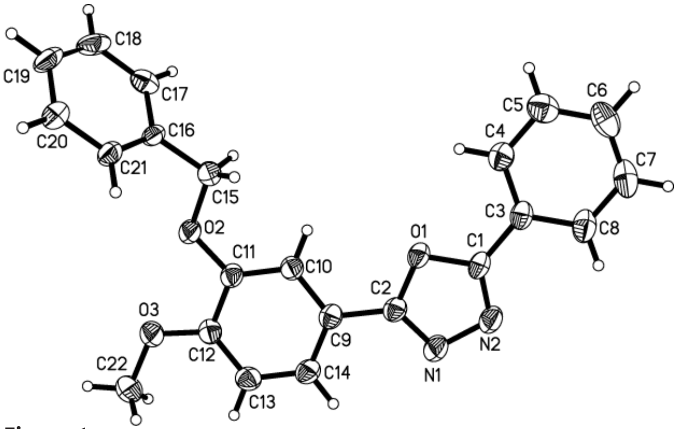


Figure 1
The molecular structure of (I). Disorder affecting the C16–C21 benzene ring has been omitted; only the major component is shown. Displacement ellipsoids are drawn at the 30% probability level.

448 K). ^{1}H NMR: δ 3.96 (*s*, 3H, O-CH$_3$), 5.24 (*s*, 2H, –CH$_2$), 6.99–8.12 (*m*, 13H, ArH). The solid (50 mg) was dissolved in ethyl acetate–petroleum ether (3:1, 30 ml) and the solution kept at room temperature for 15 d. Natural evaporation gave colourless single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{22}H_{18}N_2O_3$
$M_r = 358.38$
Triclinic, $P\overline{1}$
$a = 8.8670\ (12)$ Å
$b = 9.7248\ (13)$ Å
$c = 11.2270\ (15)$ Å
$\alpha = 101.006\ (2)^\circ$
$\beta = 105.841\ (2)^\circ$
$\gamma = 93.966\ (2)^\circ$
$V = 906.6\ (2)$ Å^3
$Z = 2$
$D_x = 1.313$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2107 reflections
$\theta = 2.4$–28.1°
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.26 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.965$, $T_{\max} = 0.983$
4966 measured reflections
3176 independent reflections
2468 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 25.0^\circ$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 7$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.104$
$S = 1.06$
3176 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.3625 (15)	N1—C2	1.2909 (17)
O1—C2	1.3587 (16)	N2—C1	1.2903 (18)
N1—N2	1.3966 (17)		
C2—O1—C1	103.08 (10)	N2—C1—O1	111.82 (12)
C2—N1—N2	106.43 (12)	N1—C2—O1	112.04 (12)
C1—N2—N1	106.62 (11)		

H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and refined using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The C16–C21 benzene ring was found to be disordered and refined over two positions [occupancies 0.750 (8) and 0.250 (8) for the unprimed and primed atoms]. During the refinement, the disordered rings were constrained to be regular hexagons with C—C distances of 1.39 Å.

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

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