Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 2-{[3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl]-methoxy}phenylacetate

Hai-Bo Wang,* Jia-Hui Chen, Yue-Qing Pu and Jin-Tang Wang

Department of Applied Chemistry, College of Science, Nanjing University of Technology, Xinmofan Road No. 5 Nanjing, Nanjing 210009, People's Republic of China

Correspondence e-mail: wanghaibo@njut.edu.cn

Received 11 October 2004
Accepted 15 October 2004
Online 22 October 2004

Key indicators

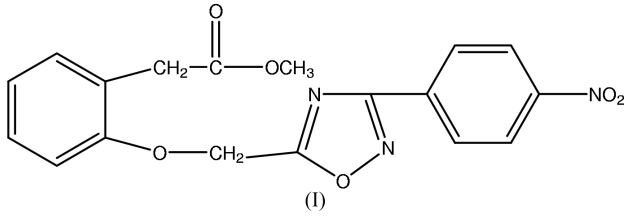
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.190
Data-to-parameter ratio = 13.6

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

The title compound, $C_{18}H_{15}N_3O_6$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 5-chloromethyl-3-(4-nitrophenyl)-1,2,4-oxadiazole. In the crystal structure, there are intermolecular C—H···N and C—H···π interactions.

Comment

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties and are efficient as agonists [*e.g.* for angiotension (Naka & Kubo, 1999) and adhesion (Juraszyk *et al.*, 1997)] for different receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angles are given in Table 1. In the crystal structure, molecules are linked by C—H···N hydrogen bonds and there is also an intermolecular contact which indicates a weak C—H···π interaction. Full details of the hydrogen bonding are given in Table 2 (see also Figs. 2 and 3). The combination of the two types of weak interaction generates a three-dimensional network.

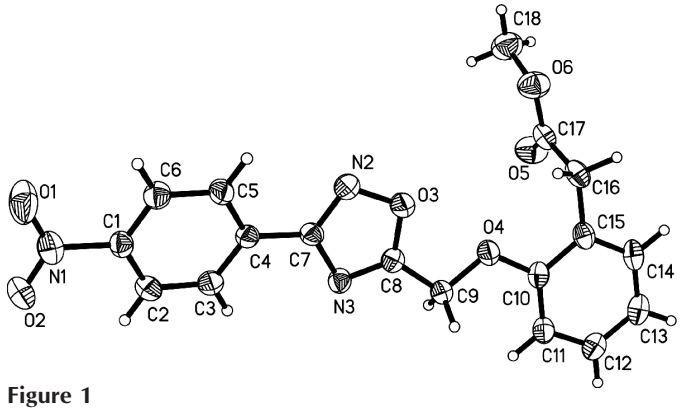


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level

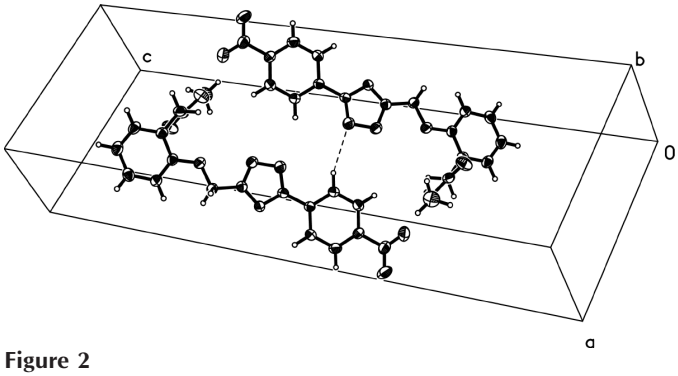


Figure 2
The short C—H···N contact (dashed line) in the crystal structure of (I).

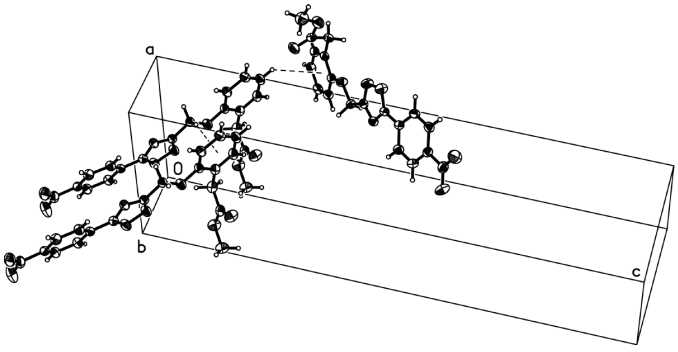


Figure 3
The C—H···π interactions in (I), shown as dashed lines.

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolve in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 5-Chloromethyl-3-(4-nitrophenyl)-1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to this mixture. The resulting mixture was refluxed for 6 h. The mixture was filtered and the filtrate concentrated under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by crystallization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 8.37–8.39 (*m*, 2H), 8.31–8.32 (*m*, 2H), 7.30–7.32 (*m*, 1H), 7.27–7.28 (*m*, 2H), 7.06–7.07 (*m*, 1H), 5.42 (*s*, 2H), 3.76 (*s*, 2H), 3.73 (*s*, 3H).

Crystal data

$C_{18}H_{15}N_3O_6$
M_r = 369.33
Monoclinic, $P2_1/c$
a = 10.436 (2) Å
b = 5.180 (1) Å
c = 31.560 (6) Å
β = 92.94 (3)°
V = 1703.8 (6) Å^3
Z = 4
D_x = 1.440 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–13°
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3538 measured reflections
3344 independent reflections
1728 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.0°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 6$
$l = -38 \rightarrow 38$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.190
S = 1.04
3344 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.007 (2)

Table 1
Selected geometric parameters (Å, °).

O3—C8	1.333 (3)	N3—C8	1.293 (4)
O3—N2	1.414 (3)	N3—C7	1.376 (4)
O4—C9	1.410 (3)	C4—C7	1.463 (4)
O4—C10	1.386 (4)	C7—N2	1.302 (4)
O6—C17	1.332 (4)	C8—C9	1.487 (4)
O6—C18	1.440 (4)	C15—C16	1.504 (4)
N1—O1	1.218 (4)	C17—O5	1.191 (4)
N1—O2	1.224 (4)	C17—C16	1.509 (4)
N1—C1	1.474 (4)		
C8—O3—N2	105.8 (2)	N3—C7—C4	123.7 (3)
C10—O4—C9	116.9 (2)	N3—C8—O3	113.7 (3)
C17—O6—C18	116.8 (3)	N3—C8—C9	126.6 (3)
O1—N1—O2	124.1 (3)	O3—C8—C9	119.5 (3)
O1—N1—C1	117.8 (3)	O4—C9—C8	107.7 (2)
O2—N1—C1	118.0 (3)	C11—C10—O4	123.8 (3)
C7—N2—O3	103.7 (2)	O4—C10—C15	114.6 (3)
C8—N3—C7	102.8 (2)	C15—C14—C13	121.9 (3)
C2—C1—N1	119.1 (3)	C14—C15—C16	122.2 (3)
C6—C1—N1	119.1 (3)	C10—C15—C16	120.3 (3)
C3—C4—C7	119.1 (3)	C15—C16—C17	114.7 (3)
C5—C4—C7	121.8 (3)	O5—C17—O6	123.3 (3)
N2—C7—N3	113.9 (3)	O5—C17—C16	126.0 (3)
N2—C7—C4	122.3 (3)	O6—C17—C16	110.7 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···N2^{i}	0.93	2.54	3.436 (4)	161
C13—H13A···$Cg3^{ii}$	0.93	3.02	3.755	137

Symmetry codes: (i) $1-x, 2-y, -z$; (ii) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$. $Cg3$ is the centroid of the C10–C15 ring.

All H atoms were positioned geometrically, with C—H distances of 0.93–0.97 Å and included in the refinement using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL*97.

References

Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD*4. University of Marburg, Germany.
Juraszyk, H., Gante, J., Wurziger, H., Bernotat-Danielowski, S. & Melzer, G. (1997). PCT Int. Appl. WO 9 744 333.
Naka, T. & Kubo, K (1999). *Curr. Pharm. Des*. **5**, 453–472.
Nicolaides, D. N., Fylaktakidou, K. C., Litinas, K. E. & Hadjipavlou-Litina, D. (1998). *Eur. J. Med. Chem.* **33**, 715–724.

Romero, J. R. (2001). *Expert Opin. Invest. Drugs*, **10**, 369–379.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Terashita, Z., Naruo, K. & Morimoto, S. (2002). PCT Int. Appl. WO 0 260 439.