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5-Chloromethyl-3-(3-methoxyphenyl)-1,2,4-oxadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.069
wR factor = 0.231
Data-to-parameter ratio = 15.2

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

In the structure of the title compound, $C_{10}H_9ClN_2O_2$, there is a weak intramolecular C—H···N interaction, and intermolecular C—H···O and C—H···N interactions.

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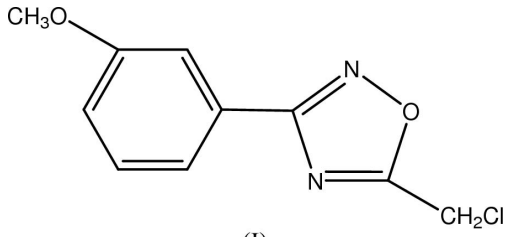
Comment

1,2,4-Oxadiazoles are an important class of five-membered heterocycle. Some derivatives of 1,2,4-oxadiazoles have shown intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties. 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. There are weak intermolecular C—H···O and C—H···N interactions (Fig. 2 and Table 2). The combination of these and a weak intramolecular C—H···N interaction generates a three-dimensional network.

Experimental

A solution of chloroacetyl chloride (14 mmol) in toluene (10 ml) was added dropwise to a solution of 3-methoxybenzamidoxime (14 mmol)

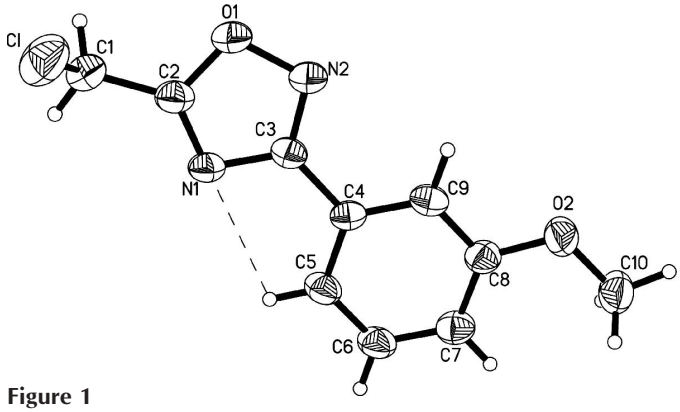


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level. The dashed line indicates the intramolecular C—H···N interaction.

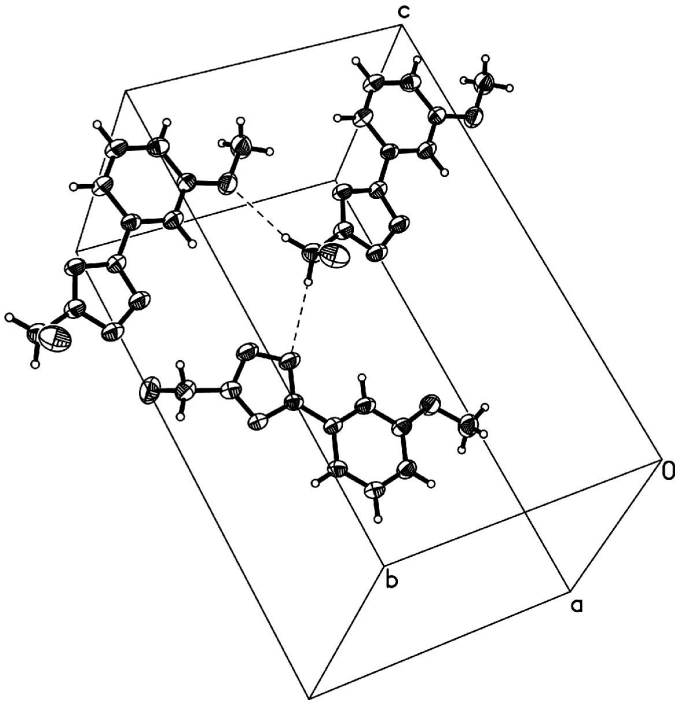


Figure 2
The crystal structure of (I). Dashed lines indicate the intermolecular C—H···O and C—H···N interactions.

in toluene (60 ml). The resulting mixture was refluxed for 6 h and then concentrated under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by recrystallization from a mixture of ethyl acetate (15 ml) and petrolum ether (7.5 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.66–7.68 (*m*, 1H), 7.59–7.60 (*m*, 1H), 7.37–7.40 (*m*, 1H), 7.05–7.07 (*m*, 1H), 4.74 (*s*, 2H), 3.87 (*s*, 3H).

Crystal data

$C_{10}H_9ClN_2O_2$
M_r = 224.64
Monoclinic, $P2_1/c$
a = 7.2350 (14) Å
b = 9.5600 (19) Å
c = 15.454 (3) Å
β = 97.03 (3)°
V = 1060.9 (4) Å^3
Z = 4
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–13°
μ = 0.34 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2234 measured reflections
2066 independent reflections
827 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.0°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 11$
$l = -18 \rightarrow 18$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.231
S = 1.01
2066 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 0.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl—C1	1.773 (6)	N1—C2	1.285 (6)
O1—C2	1.348 (6)	N1—C3	1.376 (6)
O1—N2	1.407 (6)	N2—C3	1.294 (6)
O2—C8	1.363 (6)	C1—C2	1.465 (8)
O2—C10	1.440 (6)	C3—C4	1.470 (7)
C2—O1—N2	105.8 (4)	N2—C3—N1	114.0 (5)
C8—O2—C10	117.4 (4)	N2—C3—C4	123.3 (5)
C2—N1—C3	103.3 (4)	N1—C3—C4	122.8 (4)
C3—N2—O1	104.0 (4)	C9—C4—C3	120.3 (5)
C2—C1—Cl	109.7 (4)	C5—C4—C3	120.0 (5)
N1—C2—O1	112.9 (5)	O2—C8—C9	116.2 (5)
N1—C2—C1	129.2 (5)	O2—C8—C7	124.6 (5)
O1—C2—C1	117.9 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O2^{i}	0.97	2.45	3.393 (4)	166
C1—H1C···N2^{ii}	0.97	2.54	3.471 (4)	161
C5—H5A···N1	0.93	2.60	2.912 (4)	100

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

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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