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4-[3-(Chloromethyl)-1,2,4-oxadiazol-5-yl]pyridine

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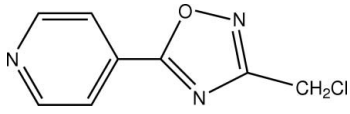
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.076; wR factor = 0.191; data-to-parameter ratio = 14.4.

In the title compound, $C_8H_6ClN_3O$, intramolecular C—H···N hydrogen bonds help to establish the molecular conformation in which the oxadiazole and pyridine rings are coplanar.

Related literature

For related literature, see: Romero (2001); Terashita *et al.* (2002).



Experimental

Crystal data

$C_8H_6ClN_3O$
M_r = 195.61
Monoclinic, $P2_1/c$
a = 10.512 (2) Å
b = 11.486 (2) Å
c = 7.2080 (14) Å
β = 94.11 (3)°
V = 868.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.924, T_{max} = 0.961
1840 measured reflections
1698 independent reflections
937 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.191
S = 1.00
1698 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1C···N3^{i}	0.97	2.58	3.522 (7)	163
C5—H5A···N1	0.93	2.61	2.924 (7)	101
C5—H5A···N2^{i}	0.93	2.54	3.316 (7)	141
C8—H8A···N2	0.93	2.58	2.892 (7)	100

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

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: *SHELXS97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2625).

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supplementary materials

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4-[3-(Chloromethyl)-1,2,4-oxadiazol-5-yl]pyridine

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Comment

1,2,4-Oxadiazole derivatives possess biological properties such as intrinsic analgesic (Terashita *et al.*, 2002) and antipicornaviral (Romero, 2001) effects. As part of out studies in this area, we report here the synthesis and crystal structure of the title compound, (I), (Fig. 1). The oxodiazole ring and its adjacent benzene ring are in the same plane [dihedral angle = 0.3 (3)°].

Two intramolecular C—H···N interactions (Table 1) help to establish the molecular conformation of (I). Two short C—H···N intermolecular contacts are also present.

Experimental

N'-hydroxyisonicotinamidine (24 mmol) was dissolved in 50 ml toluene and the mixture was cooled in an ice bath to 278 K. 2-Chloroacetyl chloride (30 mmol) in 5 ml toluene was added drop-wise. The cold bath was removed and the mixture was refluxed for 1 hr then poured into 50 ml water. 50 ml Saturated brine was added, the organic fraction was dried over anhydrous magnesium sulfate and evaporated to dryness to give the title compound (5 g). Colourless blocks of (I) were obtained by slow evaporation of an ethanol solution.

Refinement

All H atoms were placed geometrically (N—H = 0.86, C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier).

Figures

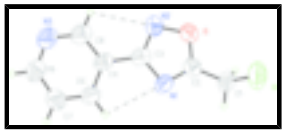


Fig. 1. A view of the molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Dashed lines indicate the hydrogen bonds.

4-(3-(Chloromethyl)-1,2,4-oxadiazol-5-yl)pyridine

Crystal data

$C_8H_6ClN_3O$	F_{000} = 400
M_r = 195.61	D_x = 1.497 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 10.512 (2) Å	θ = 9–12º

b = 11.486 (2) Å	μ = 0.40 mm^{-1}
c = 7.2080 (14) Å	T = 293 (2) K
β = 94.11 (3)º	Block, colourless
V = 868.1 (3) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Nonius CAD-4 diffractometer	R_{int} = 0.062
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.9º
T = 293(2) K	h = −12→12
ω/2θ scans	k = 0→14
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→8
T_{min} = 0.924, T_{max} = 0.961	3 standard reflections
1840 measured reflections	every 200 reflections
1698 independent reflections	intensity decay: none
937 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H-atom parameters constrained
$wR(F^2)$ = 0.191	$w = 1/[\sigma^2(F_o^2) + (0.050P)^2 + 2.350P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1698 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
118 parameters	$\Delta\rho_{min}$ = −0.36 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl	0.52306 (14)	0.64720 (16)	0.1385 (2)	0.0849 (6)
O	0.7692 (3)	0.4888 (3)	0.0884 (5)	0.0590 (10)
N1	0.8725 (4)	0.6501 (3)	0.1618 (6)	0.0554 (11)
C1	0.6560 (5)	0.6635 (5)	0.0065 (7)	0.0606 (14)
H1B	0.6353	0.6329	−0.1174	0.073*
H1C	0.6745	0.7458	−0.0055	0.073*
N2	0.8883 (4)	0.4531 (4)	0.1708 (6)	0.0600 (11)
C2	0.7692 (5)	0.6047 (5)	0.0876 (7)	0.0503 (12)
C7	1.2517 (5)	0.6678 (5)	0.4255 (9)	0.0760 (18)
H7A	1.2924	0.7383	0.4530	0.091*
C3	0.9434 (5)	0.5523 (4)	0.2100 (6)	0.0487 (11)
C4	1.0744 (5)	0.5578 (4)	0.3039 (7)	0.0500 (12)
C5	1.1302 (5)	0.6650 (4)	0.3419 (8)	0.0637 (15)
H5A	1.0865	0.7335	0.3117	0.076*
C6	1.3113 (5)	0.5643 (5)	0.4673 (8)	0.0659 (15)
H6A	1.3932	0.5676	0.5251	0.079*
N3	1.2620 (4)	0.4590 (4)	0.4320 (7)	0.0678 (13)
C8	1.1440 (5)	0.4579 (5)	0.3476 (7)	0.0617 (14)
H8A	1.1070	0.3863	0.3168	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0485 (8)	0.1060 (13)	0.0991 (12)	0.0094 (8)	−0.0030 (7)	−0.0083 (10)
O	0.055 (2)	0.053 (2)	0.067 (2)	−0.0068 (17)	−0.0027 (17)	0.0029 (17)
N1	0.054 (3)	0.048 (2)	0.063 (3)	0.011 (2)	0.001 (2)	0.006 (2)
C1	0.054 (3)	0.065 (3)	0.060 (3)	0.011 (3)	−0.011 (2)	0.001 (3)
N2	0.045 (2)	0.062 (3)	0.073 (3)	0.001 (2)	0.001 (2)	−0.001 (2)
C2	0.048 (3)	0.057 (3)	0.046 (3)	−0.004 (2)	0.005 (2)	−0.006 (2)
C7	0.054 (3)	0.063 (4)	0.110 (5)	−0.007 (3)	0.002 (3)	−0.008 (3)
C3	0.057 (3)	0.046 (3)	0.046 (3)	0.003 (2)	0.019 (2)	0.000 (2)
C4	0.048 (3)	0.045 (3)	0.060 (3)	0.008 (2)	0.017 (2)	−0.002 (2)
C5	0.051 (3)	0.046 (3)	0.093 (4)	0.002 (3)	0.004 (3)	0.004 (3)
C6	0.050 (3)	0.075 (4)	0.073 (4)	0.009 (3)	0.007 (3)	0.011 (3)
N3	0.051 (3)	0.067 (3)	0.086 (3)	0.015 (2)	0.013 (2)	−0.001 (3)
C8	0.057 (3)	0.058 (3)	0.073 (4)	0.007 (3)	0.023 (3)	−0.002 (3)

Geometric parameters (Å, °)

Cl—C1	1.756 (6)	C7—C5	1.373 (7)
O—C2	1.331 (6)	C7—H7A	0.9300
O—N2	1.408 (5)	C3—C4	1.492 (7)
N1—C2	1.286 (6)	C4—C5	1.383 (7)
N1—C3	1.379 (6)	C4—C8	1.385 (7)
C1—C2	1.454 (6)	C5—H5A	0.9300

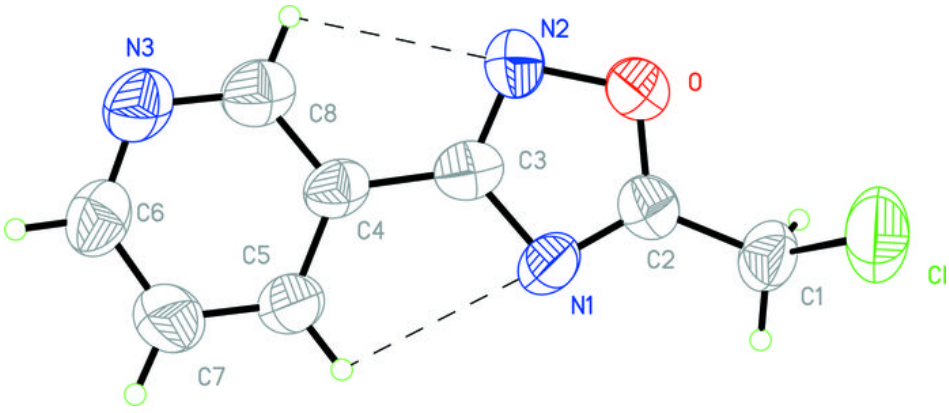
C1—H1B	0.9700	C6—N3	1.334 (7)
C1—H1C	0.9700	C6—H6A	0.9300
N2—C3	1.299 (6)	N3—C8	1.342 (7)
C7—C6	1.367 (8)	C8—H8A	0.9300
C2—O—N2	107.0 (4)	N2—C3—C4	121.2 (4)
C2—N1—C3	101.5 (4)	N1—C3—C4	123.0 (4)
C2—C1—Cl	113.1 (4)	C5—C4—C8	118.8 (5)
C2—C1—H1B	109.0	C5—C4—C3	119.5 (4)
Cl—C1—H1B	109.0	C8—C4—C3	121.6 (5)
C2—C1—H1C	109.0	C7—C5—C4	118.5 (5)
Cl—C1—H1C	109.0	C7—C5—H5A	120.8
H1B—C1—H1C	107.8	C4—C5—H5A	120.8
C3—N2—O	101.9 (4)	N3—C6—C7	125.5 (5)
N1—C2—O	113.9 (4)	N3—C6—H6A	117.2
N1—C2—C1	128.4 (5)	C7—C6—H6A	117.2
O—C2—C1	117.8 (4)	C6—N3—C8	115.4 (5)
C6—C7—C5	118.2 (6)	N3—C8—C4	123.5 (5)
C6—C7—H7A	120.9	N3—C8—H8A	118.2
C5—C7—H7A	120.9	C4—C8—H8A	118.2
N2—C3—N1	115.8 (5)		
C2—O—N2—C3	0.5 (5)	N1—C3—C4—C5	−1.4 (7)
C3—N1—C2—O	1.0 (6)	N2—C3—C4—C8	2.1 (7)
C3—N1—C2—C1	−179.3 (5)	N1—C3—C4—C8	−178.9 (5)
N2—O—C2—N1	−1.0 (6)	C6—C7—C5—C4	−0.2 (9)
N2—O—C2—C1	179.2 (4)	C8—C4—C5—C7	−1.4 (8)
Cl—C1—C2—N1	−110.7 (6)	C3—C4—C5—C7	−178.9 (5)
Cl—C1—C2—O	68.9 (5)	C5—C7—C6—N3	0.7 (10)
O—N2—C3—N1	0.1 (5)	C7—C6—N3—C8	0.3 (9)
O—N2—C3—C4	179.2 (4)	C6—N3—C8—C4	−2.0 (8)
C2—N1—C3—N2	−0.6 (6)	C5—C4—C8—N3	2.6 (8)
C2—N1—C3—C4	−179.7 (4)	C3—C4—C8—N3	−179.9 (4)
N2—C3—C4—C5	179.5 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1C···N3^{i}	0.97	2.58	3.522 (7)	163
C5—H5A···N1	0.93	2.61	2.924 (7)	101
C5—H5A···N2^{i}	0.93	2.54	3.316 (7)	141
C8—H8A···N2	0.93	2.58	2.892 (7)	100

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

Fig. 1



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4-[3-(Chloromethyl)-1,2,4-oxadiazol-5-yl]pyridine. Corrigendum

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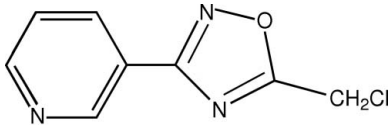
The title and the chemical diagram of the paper by Kang, Li, Zeng, Wang & Wang [*Acta Cryst.* (2007), E**63**, o4654] are corrected.

In the paper by Kang, Li, Zeng, Wang & Wang [*Acta Cryst.* (2007), E**63**, o4654], the title and the chemical diagram are incorrect. The correct structure is shown below and the correct title of the original paper should be '3-[5-(Chloromethyl)-1,2,4-oxadiazol-3-yl]pyridine'.



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