Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-5-{[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]sulfanylmethyl}pyridine

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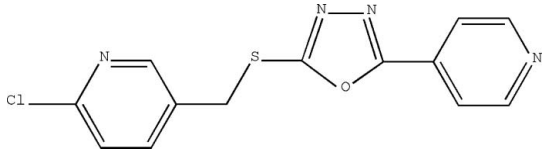
Received 12 June 2007; accepted 24 July 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.131; data-to-parameter ratio = 14.0.

In the title compound, $C_{13}H_9ClN_4OS$, the mean plane of the oxadiazole ring makes a dihedral angle of 6.34 (13)° with the mean plane of the pyridine ring. The dihedral angle between the chloropyridine ring and the oxadiazole ring is 74.43 (12)°, and the dihedral angle between the chloropyridine ring and the pyridine ring is 69.78 (11)°. The crystal packing is stabilized by inter- and intramolecular C—H···N hydrogen bonds.

Related literature

For the biological and pharmaceutical activity of oxadiazoles, see Reddy & Reddy (1987); Hui *et al.* (2000). Many derivatives of oxadiazoles have been prepared by Lin *et al.* (2002). For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_9ClN_4OS$
M_r = 304.75
Triclinic, $P\overline{1}$
a = 6.2729 (5) Å
b = 8.1448 (6) Å
c = 14.0994 (11) Å
α = 85.520 (1)°
β = 77.793 (1)°
γ = 68.637 (1)°
V = 655.70 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 297 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.877, T_{max} = 0.915
4655 measured reflections
2544 independent reflections
2108 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.131
S = 1.13
2544 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N4^{i}	0.93	2.61	3.515 (3)	164
C13—H13···N3^{ii}	0.93	2.58	3.462 (3)	158
C5—H5···N2	0.93	2.61	3.273 (3)	129
C6—H6*A*···N2	0.97	2.55	2.961 (3)	106

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 1997).

The authors gratefully acknowledge financial support of this work by the National Basic Research Programme of China (grant No. 2003CB114400) and the National Natural Science Foundation of China (grant No. 20372023).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2092).

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supplementary materials

Acta Cryst. (2007). E**63**, o3721 [**doi:10.1107/S1600536807036148**]

2-Chloro-5-{[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]sulfanylmethyl}pyridine

W.-D. Wang, Q.-Y. Ren, J.-J. Wei and H.-W. He

Comment

1,3,4,-oxadiazole derivatives are important compounds with versatile industrial and medical applications (Reddy & Reddy, 1987; Hui *et al.*, 2000; Lin *et al.*, 2002). We report here the molecular structure of (I). In the title compound, all bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and the molecules are stabilized by intra and intermolecular hydrogen bonds (Table 1). The crystal packing also shows two weak intramolecular π— π stacking interactions.

Experimental

5-Pyridin-4-yl-1,3,4-oxadiazole-2-thiol (0.72 g, 4 mmol) was added to a solution of 1.2% sodium hydroxide at room temperature while stirring. The mixture of 2-Chloro-5-chloromethyl-pyridine (0.72 g, 4.4 mmol) in methanol (4 ml) was added dropwise while the 5-Pyridin-4-yl-1,3,4-oxadiazole-2-thiol was dissolved. The mixture was then stirred at room temperature for 6 h. The white solid was filtered and recrystallized from dimethylformamide-water mixture to give the title compound (yield 54%). Colourless crystals of (I) suitable for X-ray structure analysis were grown from the mixture of dichloromethane and n-hexane (*v*/*v*, 1:8).

Refinement

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

Figures

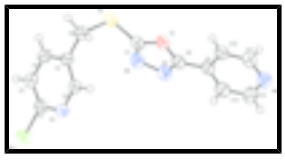

Fig. 1. The structure of (I). showing 50% probability displacement ellipsoids and the atom-numbering scheme.

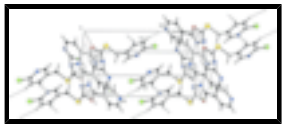

Fig. 2. Crystal Packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-Chloro-5-{[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]sulfanylmethyl}pyridine

Crystal data

$C_{13}H_9ClN_4OS$	$Z = 2$
$M_r = 304.75$	$F_{000} = 312$

Triclinic, $P\bar{1}$	D_x = 1.544 Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.2729 (5) Å	Cell parameters from 2330 reflections
b = 8.1448 (6) Å	θ = 2.7–28.2º
c = 14.0994 (11) Å	μ = 0.45 mm^{-1}
α = 85.520 (1)º	T = 297 (2) K
β = 77.793 (1)º	Block, colourless
γ = 68.637 (1)º	0.30 × 0.20 × 0.20 mm
V = 655.70 (9) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2544 independent reflections
Radiation source: fine-focus sealed tube	2108 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 297(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −7→7
T_{min} = 0.877, T_{max} = 0.915	k = −6→10
4655 measured reflections	l = −16→17

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.0355P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.131	$(\Delta/\sigma)_{max} < 0.001$
S = 1.13	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
2544 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
182 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.069 (8)
Secondary atom site location: difference Fourier map	

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}
C1	0.6614 (4)	0.2322 (3)	0.49086 (15)	0.0395 (5)
C2	0.8922 (4)	0.2144 (3)	0.47658 (17)	0.0436 (5)
H2	1.0002	0.1538	0.4234	0.052*
C3	0.9574 (4)	0.2900 (3)	0.54425 (17)	0.0435 (5)
H3	1.1120	0.2809	0.5376	0.052*
C4	0.7901 (4)	0.3801 (3)	0.62265 (15)	0.0381 (5)
C5	0.5648 (4)	0.3872 (3)	0.62834 (15)	0.0413 (5)
H5	0.4522	0.4472	0.6806	0.050*
C6	0.8574 (4)	0.4667 (3)	0.69576 (17)	0.0462 (6)
H6A	0.7238	0.5685	0.7225	0.055*
H6B	0.9804	0.5086	0.6630	0.055*
C7	0.6924 (4)	0.3411 (3)	0.86759 (16)	0.0403 (5)
C8	0.4622 (4)	0.2839 (3)	0.98761 (15)	0.0396 (5)
C9	0.3821 (4)	0.1990 (3)	1.07587 (15)	0.0390 (5)
C10	0.5377 (4)	0.0739 (3)	1.12639 (17)	0.0432 (5)
H10	0.6981	0.0388	1.1039	0.052*
C11	0.4464 (4)	0.0041 (3)	1.21055 (17)	0.0498 (6)
H11	0.5506	−0.0794	1.2438	0.060*
C12	0.0730 (5)	0.1666 (4)	1.19713 (19)	0.0543 (7)
H12	−0.0866	0.1978	1.2208	0.065*
C13	0.1458 (4)	0.2445 (3)	1.11242 (18)	0.0484 (6)
H13	0.0374	0.3265	1.0803	0.058*
Cl1	0.57259 (11)	0.14110 (9)	0.40489 (4)	0.0542 (2)
N1	0.4965 (3)	0.3144 (3)	0.56436 (13)	0.0423 (5)
N2	0.4872 (3)	0.4496 (3)	0.86157 (13)	0.0464 (5)
N3	0.3340 (3)	0.4109 (3)	0.94122 (14)	0.0448 (5)
N4	0.2198 (4)	0.0483 (3)	1.24723 (15)	0.0528 (5)
O1	0.6933 (3)	0.23080 (19)	0.94565 (10)	0.0410 (4)
S1	0.95815 (10)	0.32163 (9)	0.79527 (4)	0.0493 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0466 (13)	0.0414 (12)	0.0346 (11)	−0.0197 (10)	−0.0112 (9)	0.0048 (9)
C2	0.0417 (12)	0.0459 (13)	0.0398 (12)	−0.0155 (10)	−0.0014 (9)	0.0006 (10)
C3	0.0320 (11)	0.0519 (14)	0.0465 (13)	−0.0169 (10)	−0.0052 (9)	0.0042 (10)
C4	0.0408 (12)	0.0415 (12)	0.0377 (11)	−0.0209 (10)	−0.0115 (9)	0.0084 (9)
C5	0.0371 (12)	0.0518 (14)	0.0350 (11)	−0.0178 (10)	−0.0037 (9)	−0.0008 (10)
C6	0.0481 (14)	0.0538 (15)	0.0465 (13)	−0.0282 (12)	−0.0147 (10)	0.0070 (11)

C7	0.0468 (13)	0.0399 (12)	0.0362 (11)	−0.0138 (10)	−0.0145 (9)	−0.0022 (9)
C8	0.0436 (12)	0.0373 (12)	0.0374 (12)	−0.0111 (10)	−0.0108 (9)	−0.0068 (9)
C9	0.0432 (12)	0.0385 (12)	0.0364 (11)	−0.0131 (9)	−0.0104 (9)	−0.0068 (9)
C10	0.0390 (12)	0.0475 (13)	0.0416 (12)	−0.0116 (10)	−0.0096 (9)	−0.0047 (10)
C11	0.0596 (15)	0.0462 (14)	0.0418 (13)	−0.0143 (12)	−0.0149 (11)	0.0011 (10)
C12	0.0505 (15)	0.0587 (16)	0.0504 (15)	−0.0190 (12)	−0.0013 (11)	−0.0070 (12)
C13	0.0478 (14)	0.0460 (14)	0.0498 (14)	−0.0114 (11)	−0.0144 (11)	−0.0034 (11)
Cl1	0.0654 (4)	0.0628 (4)	0.0448 (4)	−0.0320 (3)	−0.0145 (3)	−0.0048 (3)
N1	0.0397 (10)	0.0537 (12)	0.0382 (10)	−0.0224 (9)	−0.0078 (8)	0.0007 (9)
N2	0.0459 (11)	0.0469 (11)	0.0412 (11)	−0.0091 (9)	−0.0120 (9)	0.0015 (9)
N3	0.0388 (10)	0.0503 (12)	0.0392 (10)	−0.0081 (9)	−0.0082 (8)	−0.0013 (9)
N4	0.0583 (13)	0.0546 (13)	0.0471 (12)	−0.0232 (11)	−0.0069 (10)	−0.0040 (10)
O1	0.0416 (9)	0.0421 (9)	0.0377 (8)	−0.0112 (7)	−0.0114 (6)	0.0007 (7)
S1	0.0399 (4)	0.0629 (4)	0.0474 (4)	−0.0184 (3)	−0.0153 (3)	0.0045 (3)

Geometric parameters (Å, °)

C1—N1	1.320 (3)	C7—S1	1.720 (2)
C1—C2	1.374 (3)	C8—N3	1.286 (3)
C1—Cl1	1.748 (2)	C8—O1	1.364 (3)
C2—C3	1.377 (3)	C8—C9	1.461 (3)
C2—H2	0.9300	C9—C13	1.381 (3)
C3—C4	1.392 (3)	C9—C10	1.398 (3)
C3—H3	0.9300	C10—C11	1.380 (3)
C4—C5	1.378 (3)	C10—H10	0.9300
C4—C6	1.501 (3)	C11—N4	1.328 (3)
C5—N1	1.335 (3)	C11—H11	0.9300
C5—H5	0.9300	C12—N4	1.341 (3)
C6—S1	1.826 (2)	C12—C13	1.378 (4)
C6—H6A	0.9700	C12—H12	0.9300
C6—H6B	0.9700	C13—H13	0.9300
C7—N2	1.285 (3)	N2—N3	1.412 (3)
C7—O1	1.365 (3)		
N1—C1—C2	125.6 (2)	N3—C8—O1	112.8 (2)
N1—C1—Cl1	116.04 (17)	N3—C8—C9	126.5 (2)
C2—C1—Cl1	118.31 (18)	O1—C8—C9	120.72 (17)
C1—C2—C3	117.3 (2)	C13—C9—C10	118.2 (2)
C1—C2—H2	121.3	C13—C9—C8	119.7 (2)
C3—C2—H2	121.3	C10—C9—C8	122.1 (2)
C2—C3—C4	119.5 (2)	C11—C10—C9	118.1 (2)
C2—C3—H3	120.3	C11—C10—H10	120.9
C4—C3—H3	120.3	C9—C10—H10	120.9
C5—C4—C3	117.2 (2)	N4—C11—C10	124.3 (2)
C5—C4—C6	122.8 (2)	N4—C11—H11	117.8
C3—C4—C6	120.1 (2)	C10—C11—H11	117.8
N1—C5—C4	124.8 (2)	N4—C12—C13	123.5 (2)
N1—C5—H5	117.6	N4—C12—H12	118.2
C4—C5—H5	117.6	C13—C12—H12	118.2
C4—C6—S1	113.78 (16)	C12—C13—C9	119.0 (2)

C4—C6—H6A	108.8	C12—C13—H13	120.5
S1—C6—H6A	108.8	C9—C13—H13	120.5
C4—C6—H6B	108.8	C1—N1—C5	115.59 (19)
S1—C6—H6B	108.8	C7—N2—N3	105.74 (18)
H6A—C6—H6B	107.7	C8—N3—N2	106.27 (17)
N2—C7—O1	113.2 (2)	C11—N4—C12	116.8 (2)
N2—C7—S1	129.65 (19)	C8—O1—C7	102.04 (16)
O1—C7—S1	117.16 (15)	C7—S1—C6	99.33 (11)
N1—C1—C2—C3	−0.6 (3)	C8—C9—C13—C12	−178.3 (2)
Cl1—C1—C2—C3	178.82 (16)	C2—C1—N1—C5	1.0 (3)
C1—C2—C3—C4	−0.2 (3)	Cl1—C1—N1—C5	−178.40 (16)
C2—C3—C4—C5	0.5 (3)	C4—C5—N1—C1	−0.7 (3)
C2—C3—C4—C6	−178.6 (2)	O1—C7—N2—N3	−0.4 (3)
C3—C4—C5—N1	−0.1 (3)	S1—C7—N2—N3	−178.04 (18)
C6—C4—C5—N1	179.0 (2)	O1—C8—N3—N2	−0.4 (2)
C5—C4—C6—S1	92.6 (2)	C9—C8—N3—N2	179.6 (2)
C3—C4—C6—S1	−88.4 (2)	C7—N2—N3—C8	0.5 (2)
N3—C8—C9—C13	5.5 (4)	C10—C11—N4—C12	1.1 (4)
O1—C8—C9—C13	−174.5 (2)	C13—C12—N4—C11	−1.2 (4)
N3—C8—C9—C10	−173.4 (2)	N3—C8—O1—C7	0.2 (2)
O1—C8—C9—C10	6.6 (3)	C9—C8—O1—C7	−179.87 (19)
C13—C9—C10—C11	−0.7 (3)	N2—C7—O1—C8	0.2 (2)
C8—C9—C10—C11	178.3 (2)	S1—C7—O1—C8	178.12 (15)
C9—C10—C11—N4	−0.2 (4)	N2—C7—S1—C6	−11.0 (2)
N4—C12—C13—C9	0.4 (4)	O1—C7—S1—C6	171.46 (17)
C10—C9—C13—C12	0.6 (4)	C4—C6—S1—C7	−82.18 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N4^{i}	0.93	2.61	3.515 (3)	164
C13—H13···N3^{ii}	0.93	2.58	3.462 (3)	158
C5—H5···N2	0.93	2.61	3.273 (3)	129
C6—H6A···N2	0.97	2.55	2.961 (3)	106

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

Fig. 1

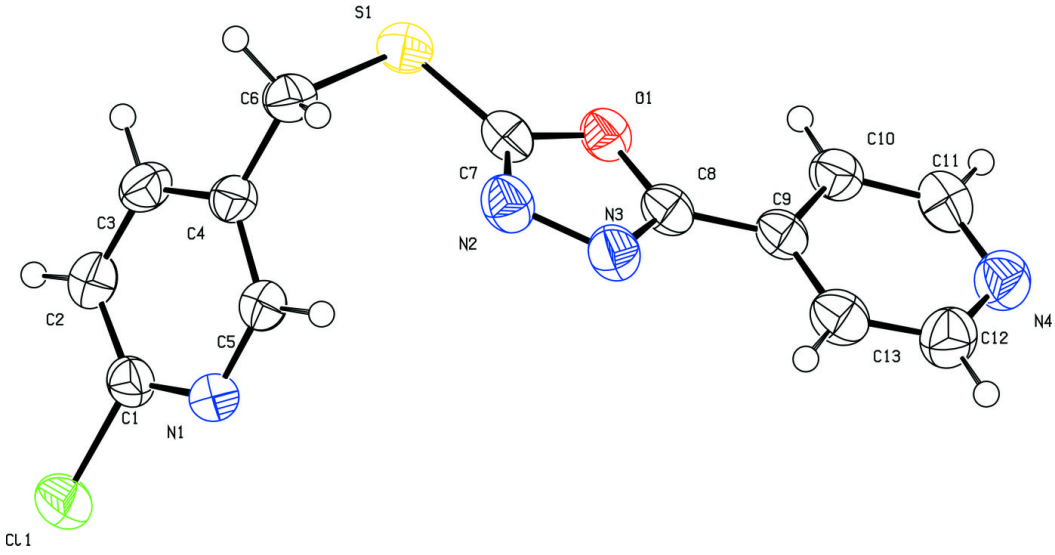

Fig. 2