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(*Z*)-3-(2,6-Dichlorophenyl)-1-(pyridin-3-yl)-2-(1*H*-1,2,4-triazol-1-yl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.087
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.

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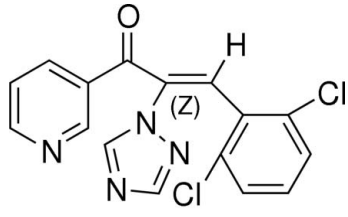
The title compound, $C_{16}H_{10}Cl_2N_4O$, has been synthesized as a potent fungicidal agent and plant growth regulatory agent, and its crystal structure was determined. In the crystal structure, weak intermolecular C—H···Cl interactions are found. The dihedral angles between the planes of the pyridine and triazole rings, and between the substituted phenyl and triazole rings, are 82.4 (2) and 118.8 (3)°, respectively.

Comment

It is well known that compounds containing 1*H*-1,2,4-triazole ring systems have good biological and physiological activities. The agrochemicals triadimefon, triadimenol, flusilazole and cyproconazole (Frohberger, 1978; Wackers *et al.*, 1978; Hu *et al.*, 2004), and clinical drugs fluconazole and itraconazole (Haria *et al.*, 1996; Goa & Barradell, 1996) are a class of biologically significant compounds which have been widely used as antifungal agents against mildews and rusts of cereal grains, fruits, vegetables and ornamentals. (Koltin & Hitchcock, 1997). These compounds are known as potent inhibitors of cytochrome P450 monooxygenase in the process of the fungal biosynthesis of ergosterol P450, an important enzyme in ergosterol biosynthesis in fungi and cholesterol synthesis in mammalian cells (Fang *et al.*., 2003; Kapteyn *et al.*, 1992; Hiroshi *et al.*, 1995).

Pyridine derivatives not only possess high biological activities but also have better solubility, lower toxicity and higher selectivity. In order to obtain unexpected biologically active compounds, the pyridinyl group has often been incorporated into organic molecules (Friesen *et al.*, 1998; Dube *et al.*, 1999; Bis *et al.*, 1998; Kurahashi *et al.*, 1997; Schallner *et al.*, 2000; Ife *et al.*., 1995; Xiong *et al.*, 2001; Zhao *et al.*, 2004). Encouraged by these studies, we incorporated the pyridinyl unit into the title triazole, (I). We report here the crystal structure of (I).



(I)

Fig. 1 shows the molecular structure of (I), which contains three planar rings: the pyridinyl ring (*p*1), the triazole ring (*p*2) and the substituted phenyl ring (*p*3). The dihedral angles between *p*1 and *p*2, and between *p*3 and *p*2, are 82.4 (2) and 118.8 (3)°, respectively. In the crystal structure, weak inter-

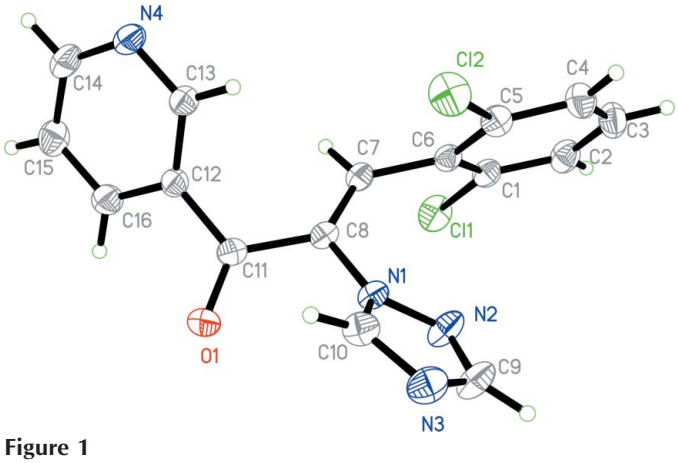


Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level.

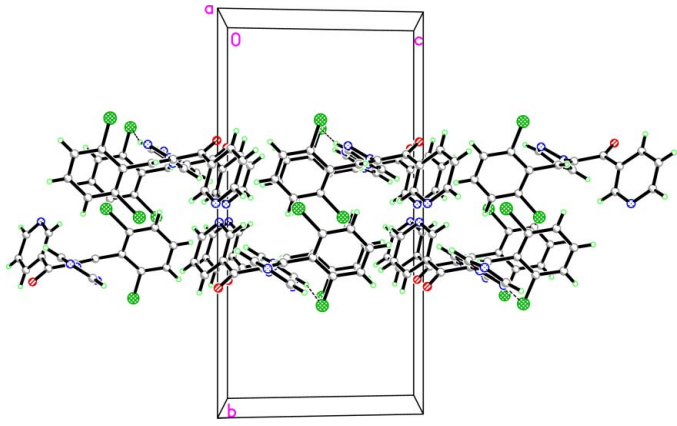


Figure 2
Packing diagram of (I). Dashed lines indicate C–H···Cl hydrogen-bond interactions.

molecular C—H···Cl interactions are found [C9—H9···Cl1^{i}; C—H = 0.93 Å, H···Cl = 2.849 Å, C···Cl = 3.689 (1) Å and C—H···Cl = 151°; symmetry code: (i) $x-1, y, z$] (Fig. 2).

Experimental

To a stirred solution of 1-(pyridin-3-yl)-2-(1*H*-1,2,4-triazol-1-yl)-ethanone (1.00 g, 3.83 mmol), 2,6-dichlorobenzaldehyde (1.12 g, 4.60 mmol) and dry chloroform (30 ml) were added a few drops of piperidine at room temperature under nitrogen. The mixture was heated to reflux for 4 h. The solvent was evaporated under reduced pressure, and the residue was then purified by column chromatography on silica gel (200–300 mesh) with petroleum ether/ethyl acetate (4:1 *v*/*v*) as eluant; the resulting white solid was recrystallized from petroleum ether/ethyl acetate (3:1 *v*/*v*) to give white crystals (yield 50.0%).

Crystal data

$C_{16}H_{10}Cl_2N_4O$
$M_r = 345.18$
Monoclinic, $P2_1/n$
$a = 8.0749\ (14)$ Å
$b = 19.795\ (3)$ Å
$c = 10.1321\ (17)$ Å
$\beta = 98.280\ (2)°$
$V = 1602.7\ (5)$ Å^3
$Z = 4$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2848 reflections
$\theta = 2.3–23.8°$
$\mu = 0.41$ mm^{-1}
$T = 294\ (2)$ K
Block, white
0.46 × 0.32 × 0.18 mm

Data collection

Bruker SMART APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.760$, $T_{max} = 0.928$
8638 measured reflections
2837 independent reflections
2308 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$
$h = -9 \rightarrow 9$
$k = -23 \rightarrow 22$
$l = -10 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.087$
$S = 1.08$
2837 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.2713P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.7292 (17)	N3—C10	1.306 (2)
Cl2—C5	1.7373 (17)	N4—C13	1.330 (2)
O1—C11	1.212 (2)	C5—C6	1.392 (2)
N1—C10	1.339 (2)	C6—C7	1.475 (2)
N1—N2	1.3608 (19)	C7—C8	1.328 (2)
N1—C8	1.418 (2)		
C10—N1—N2	108.82 (14)	C7—C8—N1	121.81 (15)
C10—N1—C8	129.33 (14)	C7—C8—C11	123.08 (15)
N2—N1—C8	121.82 (13)	N1—C8—C11	114.82 (13)
C10—N3—C9	101.71 (15)	N2—C9—N3	116.27 (17)
C13—N4—C14	116.31 (16)	N3—C10—N1	111.37 (16)
C2—C1—Cl1	118.68 (13)	O1—C11—C12	120.06 (15)
C6—C1—Cl1	118.86 (13)	O1—C11—C8	120.44 (15)
C4—C5—Cl2	118.20 (14)	C12—C11—C8	119.49 (14)
C6—C5—Cl2	119.62 (13)	C16—C12—C13	118.07 (15)
C1—C6—C5	116.28 (15)	C16—C12—C11	119.77 (15)
C1—C6—C7	120.78 (14)	C13—C12—C11	121.88 (15)
C5—C6—C7	122.92 (14)	N4—C13—C12	124.03 (16)
C8—C7—C6	126.28 (15)	N4—C14—C15	124.48 (18)
C10—N1—N2—C9	−0.66 (19)	N2—N1—C8—C7	−40.2 (2)
C8—N1—N2—C9	177.43 (16)	C10—N1—C8—C11	−48.6 (2)
Cl1—C1—C2—C3	179.20 (15)	N2—N1—C8—C11	133.78 (16)
C3—C4—C5—Cl2	179.69 (14)	C8—N1—C10—N3	−176.90 (15)
Cl1—C1—C6—C5	179.91 (12)	C7—C8—C11—O1	152.18 (18)
C2—C1—C6—C7	179.26 (16)	N1—C8—C11—O1	−21.7 (2)
Cl1—C1—C6—C7	−1.6 (2)	C7—C8—C11—C12	−28.4 (2)
Cl2—C5—C6—C1	179.72 (12)	N1—C8—C11—C12	157.68 (14)
C4—C5—C6—C7	−177.73 (16)	O1—C11—C12—C16	−34.3 (3)
Cl2—C5—C6—C7	1.2 (2)	C8—C11—C12—C16	146.31 (16)
C1—C6—C7—C8	113.59 (19)	O1—C11—C12—C13	139.53 (18)
C5—C6—C7—C8	−68.0 (2)	C8—C11—C12—C13	−39.9 (2)
C6—C7—C8—N1	−5.4 (3)	C11—C12—C13—N4	−172.69 (16)
C6—C7—C8—C11	−178.94 (15)	C11—C12—C16—C15	174.68 (16)
C10—N1—C8—C7	137.44 (18)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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,1999); software used to prepare material for publication: *SHELXTL*.

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