Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Chlorophenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.115
Data-to-parameter ratio = 13.5

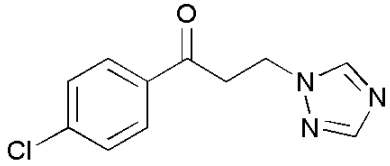
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 November 2004
Accepted 16 November 2004
Online 27 November 2004

The title compound, $C_{11}H_{10}ClN_3O$, crystallizes in space group $P\overline{1}$ with two independent molecules in the asymmetric unit. The bond lengths and angles in both molecules are within normal ranges. The dihedral angles between the planes of the triazole and benzene rings in the two independent molecules are 82.6 (1) and 85.9 (1)°.

Comment

As an important type of fungicide, triazole compounds possessing low toxicity are highly efficient (Shi *et al.*, 1995; Xu *et al.*, 2002). At present, studies of triazole derivatives are mainly concentrated on compounds with triazole as the only active group. Many highly fungicidal triazole compounds have been synthesized, including the title compound, (I) (Ogata *et al.*, 1987). We report here the crystal structure of (I).



(I)

Compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1). All bond lengths and angles in both molecules are normal (Table 1) and comparable to those in published structures (Ji *et al.*, 2002; Liu *et al.*, 2002). The

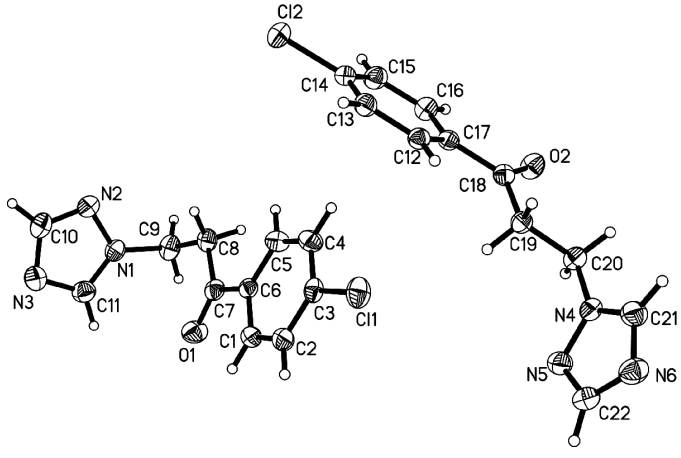


Figure 1
A view of the asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level.

dihedral angles between the planes of the triazole and benzene rings in the two independent molecules are 82.6 (1) and 85.9 (1)°. This geometry is very similar to that found in the related compounds 2-[(*p*-methoxyphenylcarbonyl)(1,2,4-triazol-1-yl)methyl]sulfanyl-4,6-dimethylpyrimidine (Jian *et al.*, 2003), 2-(1,3-dithiolan-2-ylidene)-1-phenyl-2-(1,2,4-triazol-1-yl)ethanone (Jian *et al.*, 2004) and 1-(4-fluorophenyl)-2-(3-phenylthiazolidin-2-ylidene)-2-(1*H*-1,2,4-triazol-1-yl)ethanone (Xu *et al.*, 2004).

Experimental

The title compound was prepared according to the method reported by Ogata *et al.* (1987) and crystallized from a mixture of EtOH–petroleum ether.

Crystal data

$C_{11}H_{10}ClN_3O$
M_r = 235.67
Triclinic, $P\overline{1}$
a = 10.1244 (19) Å
b = 10.571 (2) Å
c = 11.508 (2) Å
α = 95.838 (3)°
β = 107.625 (3)°
γ = 104.906 (3)°
V = 1112.6 (4) Å^3
Z = 4
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2229 reflections
θ = 2.5–25.7°
μ = 0.32 mm^{-1}
T = 293 (2) K
Prism, colorless
0.20 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.904, T_{max} = 0.962
5862 measured reflections
3905 independent reflections
2846 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°
$h = -9 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.03
3905 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.3475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.219 (3)	N4—C21	1.325 (3)
N1—C11	1.324 (3)	N4—N5	1.354 (3)
N1—N2	1.354 (3)	N4—C20	1.457 (3)
N2—C10	1.313 (3)	N5—C22	1.308 (3)
N3—C11	1.319 (3)	N6—C21	1.311 (3)
N3—C10	1.339 (4)	N6—C22	1.343 (3)
C6—C7	1.488 (3)	C17—C18	1.498 (3)
C8—C9	1.513 (4)	C18—C19	1.494 (3)
O2—C18	1.216 (3)	C19—C20	1.509 (3)
C11—N1—N2	109.2 (2)	C21—N4—N5	108.9 (2)
C11—N1—C9	130.1 (2)	C21—N4—C20	129.7 (2)
N2—N1—C9	120.6 (2)	N5—N4—C20	121.3 (2)
C10—N2—N1	101.6 (2)	C22—N5—N4	102.2 (2)
C11—N3—C10	101.2 (2)	C21—N6—C22	101.8 (2)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

This project was supported by the Natural Science Foundation of Shandong Province (grant No. Y2002B06).

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