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

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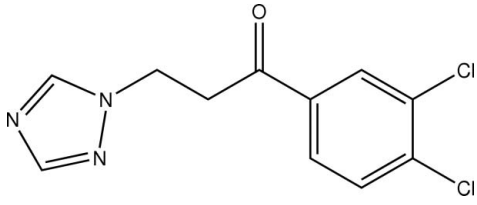
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.108; data-to-parameter ratio = 14.2.

The molecule of the title compound, $C_{11}H_9Cl_2N_3O$, is nonplanar, with a dihedral angle of 80.04 (11)° between the benzene and triazole rings. The packing is stabilized by π–π interactions, with centroid–centroid distances of 3.724 and 3.590 Å for the triazole and benzene rings, respectively, and by van der Waals forces.

Related literature

For related literature, see: Wan *et al.* (2005); Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_9Cl_2N_3O$
M_r = 270.11
Triclinic, $P\overline{1}$
a = 6.8296 (10) Å
b = 7.1403 (11) Å
c = 12.3933 (19) Å
α = 80.830 (2)°
β = 78.724 (2)°
γ = 75.612 (2)°
V = 570.19 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 293 (2) K
0.27 × 0.27 × 0.07 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.865, T_{max} = 0.962
3183 measured reflections
2194 independent reflections
1955 reflections with $I > 2\sigma(I)$
R_{int} = 0.009

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.108
S = 0.66
2194 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2305).

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supplementary materials

Acta Cryst. (2007). E**63**, o3063 [**doi:10.1107/S1600536807026207**]

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

T.-D. Li, N.-N. Tian, S. Bi and J. Wan

Comment

As part of our ongoing studies on triazole compounds, the title compound, (I), was obtained by the reaction of triazole and 1-(3,4-dichlorophenyl)-3-(dimethylamino)propan-1-one hydrochloride. We reports the crystal structure of (I) here.

All the bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The whole molecule is non-planar with a dihedral angle of 80.04 (11)° between the benzene ring (C1—C6) and triazole ring (N1—N3/C10/C11). The crystal packing is further stabilized by Van der Waals forces. The short distances $Cg1\cdots Cg1^{i}$ (3.724 Å) and $Cg2\cdots Cg2^{ii}$ (3.590 Å) [symmetry code: (i) $2-x, 1-y, 3-z$; (ii)$1-x, 1-y, 2-z$], where $Cg1$ and $Cg2$ denote the centroids of triazole ring and benzene ring, respectively, indicate π-π interactions.

Experimental

The title compound (I) was prepared according to the literature method of Wan *et al.* (2005). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 5 d.

Refinement

The H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2\ U_{eq}(C)$.

Figures

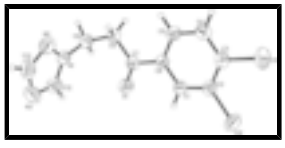

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

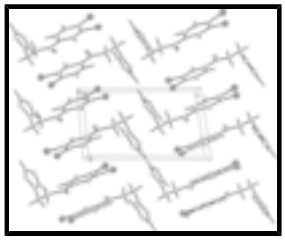

Fig. 2. Packing diagram of (I) viewed down the *a* axis.

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

Crystal data

$C_{11}H_9Cl_2N_3O$	$Z = 2$
$M_r = 270.11$	$F_{000} = 276$
Triclinic, $P\overline{1}$	$D_x = 1.573$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8296$ (10) Å	Cell parameters from 1835 reflections
$b = 7.1403$ (11) Å	$\theta = 3.1$–26.0º
$c = 12.3933$ (19) Å	$\mu = 0.55$ mm^{-1}
$\alpha = 80.830$ (2)º	$T = 293$ (2) K
$\beta = 78.724$ (2)º	Plate, colourless
$\gamma = 75.612$ (2)º	0.27 × 0.27 × 0.07 mm
$V = 570.19$ (15) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2194 independent reflections
Radiation source: fine-focus sealed tube	1955 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.009$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 1.7$º
ω scans	$h = -8 \rightarrow 4$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -8 \rightarrow 8$
$T_{min} = 0.865$, $T_{max} = 0.962$	$l = -15 \rightarrow 15$
3183 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.1029P)^2 + 0.463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.66$	$(\Delta/\sigma)_{max} = 0.001$
2194 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.22$ 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
Cl1	0.21802 (8)	0.95267 (7)	0.80256 (4)	0.05716 (19)
Cl2	0.70100 (8)	0.87272 (8)	0.76018 (4)	0.05845 (19)
C6	0.5728 (3)	0.6771 (2)	1.08034 (13)	0.0355 (4)
O1	0.8822 (2)	0.5501 (2)	1.15061 (11)	0.0532 (4)
N1	0.8075 (2)	0.6065 (2)	1.40105 (12)	0.0443 (4)
C5	0.3598 (3)	0.7133 (2)	1.09772 (15)	0.0406 (4)
H5A	0.2892	0.6815	1.1677	0.049*
C1	0.6769 (3)	0.7250 (2)	0.97532 (14)	0.0382 (4)
H1A	0.8193	0.6996	0.9626	0.046*
C4	0.2519 (3)	0.7961 (3)	1.01167 (16)	0.0437 (4)
H4A	0.1098	0.8179	1.0237	0.052*
C7	0.6964 (3)	0.5855 (2)	1.17056 (14)	0.0377 (4)
C8	0.5837 (3)	0.5375 (3)	1.28599 (14)	0.0403 (4)
H8A	0.5045	0.4433	1.2833	0.048*
H8B	0.4885	0.6546	1.3096	0.048*
C3	0.3558 (3)	0.8462 (2)	0.90829 (15)	0.0396 (4)
C2	0.5691 (3)	0.8107 (2)	0.88940 (14)	0.0394 (4)
C9	0.7250 (3)	0.4561 (3)	1.37097 (15)	0.0438 (4)
H9A	0.6499	0.3970	1.4368	0.053*
H9B	0.8371	0.3554	1.3411	0.053*
N2	0.6857 (3)	0.7499 (3)	1.45984 (14)	0.0580 (5)
C12	0.9975 (3)	0.6333 (4)	1.37805 (17)	0.0594 (6)
H12A	1.1073	0.5521	1.3389	0.071*
N3	1.0108 (4)	0.7888 (3)	1.41752 (17)	0.0744 (6)
C13	0.8161 (5)	0.8543 (4)	1.46695 (18)	0.0689 (7)
H13A	0.7768	0.9653	1.5034	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0636 (3)	0.0552 (3)	0.0515 (3)	−0.0020 (2)	−0.0247 (2)	−0.0020 (2)
Cl2	0.0628 (3)	0.0730 (4)	0.0343 (3)	−0.0149 (3)	−0.0007 (2)	−0.0001 (2)

C6	0.0395 (9)	0.0339 (8)	0.0350 (8)	−0.0110 (7)	−0.0055 (7)	−0.0059 (6)
O1	0.0388 (7)	0.0748 (9)	0.0416 (7)	−0.0087 (6)	−0.0049 (5)	−0.0029 (6)
N1	0.0470 (8)	0.0567 (9)	0.0315 (7)	−0.0195 (7)	−0.0074 (6)	0.0019 (6)
C5	0.0390 (9)	0.0425 (9)	0.0395 (9)	−0.0127 (7)	−0.0030 (7)	−0.0014 (7)
C1	0.0382 (9)	0.0403 (8)	0.0374 (9)	−0.0108 (7)	−0.0046 (7)	−0.0076 (7)
C4	0.0384 (9)	0.0426 (9)	0.0501 (10)	−0.0096 (7)	−0.0084 (8)	−0.0033 (7)
C7	0.0395 (9)	0.0397 (8)	0.0352 (9)	−0.0104 (7)	−0.0056 (7)	−0.0069 (7)
C8	0.0402 (9)	0.0454 (9)	0.0368 (9)	−0.0138 (7)	−0.0048 (7)	−0.0040 (7)
C3	0.0465 (9)	0.0323 (8)	0.0418 (9)	−0.0062 (7)	−0.0140 (7)	−0.0057 (6)
C2	0.0488 (10)	0.0364 (8)	0.0339 (8)	−0.0128 (7)	−0.0036 (7)	−0.0062 (6)
C9	0.0467 (10)	0.0476 (10)	0.0368 (9)	−0.0132 (8)	−0.0067 (7)	−0.0001 (7)
N2	0.0692 (11)	0.0622 (10)	0.0461 (9)	−0.0237 (9)	−0.0020 (8)	−0.0116 (8)
C12	0.0520 (11)	0.0837 (15)	0.0460 (11)	−0.0293 (11)	−0.0127 (9)	0.0109 (10)
N3	0.0877 (15)	0.0959 (15)	0.0591 (12)	−0.0577 (13)	−0.0323 (11)	0.0180 (11)
C13	0.109 (2)	0.0717 (14)	0.0412 (11)	−0.0455 (14)	−0.0217 (12)	0.0023 (10)

Geometric parameters (Å, °)

Cl1—C3	1.7291 (17)	C4—H4A	0.9300
Cl2—C2	1.7262 (17)	C7—C8	1.517 (2)
C6—C5	1.392 (2)	C8—C9	1.517 (3)
C6—C1	1.391 (2)	C8—H8A	0.9700
C6—C7	1.501 (2)	C8—H8B	0.9700
O1—C7	1.214 (2)	C3—C2	1.394 (3)
N1—C12	1.328 (3)	C9—H9A	0.9700
N1—N2	1.359 (2)	C9—H9B	0.9700
N1—C9	1.456 (2)	N2—C13	1.319 (3)
C5—C4	1.385 (3)	C12—N3	1.312 (3)
C5—H5A	0.9300	C12—H12A	0.9300
C1—C2	1.387 (2)	N3—C13	1.352 (4)
C1—H1A	0.9300	C13—H13A	0.9300
C4—C3	1.377 (3)		
C5—C6—C1	119.26 (16)	C9—C8—H8B	108.9
C5—C6—C7	122.57 (15)	H8A—C8—H8B	107.7
C1—C6—C7	118.17 (15)	C4—C3—C2	120.29 (16)
C12—N1—N2	109.21 (18)	C4—C3—Cl1	119.09 (14)
C12—N1—C9	129.46 (19)	C2—C3—Cl1	120.62 (14)
N2—N1—C9	121.32 (15)	C1—C2—C3	119.74 (16)
C6—C5—C4	120.62 (16)	C1—C2—Cl2	119.54 (14)
C6—C5—H5A	119.7	C3—C2—Cl2	120.72 (14)
C4—C5—H5A	119.7	N1—C9—C8	111.80 (15)
C2—C1—C6	120.24 (16)	N1—C9—H9A	109.3
C2—C1—H1A	119.9	C8—C9—H9A	109.3
C6—C1—H1A	119.9	N1—C9—H9B	109.3
C3—C4—C5	119.83 (17)	C8—C9—H9B	109.3
C3—C4—H4A	120.1	H9A—C9—H9B	107.9
C5—C4—H4A	120.1	C13—N2—N1	102.01 (19)
O1—C7—C6	120.27 (15)	N1—C12—N3	111.4 (2)
O1—C7—C8	121.24 (15)	N1—C12—H12A	124.3

C6—C7—C8	118.48 (14)	N3—C12—H12A	124.3
C7—C8—C9	113.41 (15)	C12—N3—C13	102.06 (19)
C7—C8—H8A	108.9	N2—C13—N3	115.3 (2)
C9—C8—H8A	108.9	N2—C13—H13A	122.4
C7—C8—H8B	108.9	N3—C13—H13A	122.4
C1—C6—C5—C4	0.0 (2)	C4—C3—C2—C1	−0.1 (2)
C7—C6—C5—C4	−179.28 (15)	Cl1—C3—C2—C1	−179.96 (12)
C5—C6—C1—C2	1.0 (2)	C4—C3—C2—Cl2	179.98 (13)
C7—C6—C1—C2	−179.72 (14)	Cl1—C3—C2—Cl2	0.1 (2)
C6—C5—C4—C3	−1.0 (3)	C12—N1—C9—C8	−110.1 (2)
C5—C6—C7—O1	177.26 (16)	N2—N1—C9—C8	68.8 (2)
C1—C6—C7—O1	−2.0 (2)	C7—C8—C9—N1	73.91 (19)
C5—C6—C7—C8	−2.3 (2)	C12—N1—N2—C13	0.3 (2)
C1—C6—C7—C8	178.48 (14)	C9—N1—N2—C13	−178.74 (16)
O1—C7—C8—C9	3.7 (2)	N2—N1—C12—N3	−0.5 (2)
C6—C7—C8—C9	−176.79 (14)	C9—N1—C12—N3	178.46 (17)
C5—C4—C3—C2	1.1 (3)	N1—C12—N3—C13	0.4 (2)
C5—C4—C3—Cl1	−179.07 (13)	N1—N2—C13—N3	−0.1 (2)
C6—C1—C2—C3	−0.9 (2)	C12—N3—C13—N2	−0.2 (3)
C6—C1—C2—Cl2	178.97 (12)		

Fig. 1

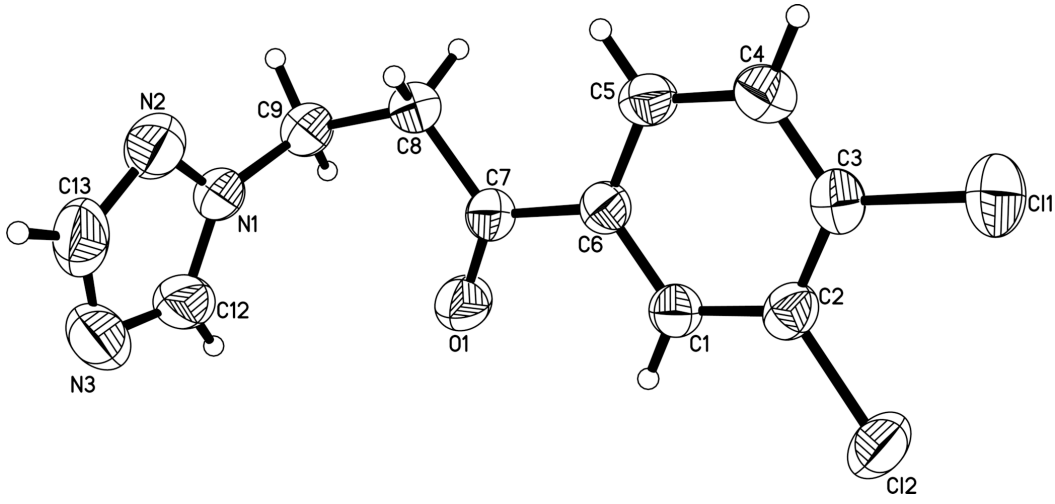

Fig. 2