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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.123
Data-to-parameter ratio = 11.3

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

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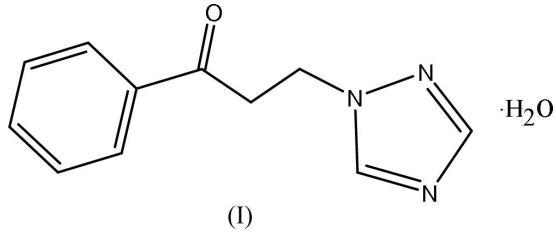
In the title compound, $C_{11}H_{11}N_3O\cdot0.5H_2O$, the dihedral angle between the two aromatic rings is 87.12 (10)°. The molecules are linked into chains along the *c* axis by intermolecular C—H···N hydrogen bonds. The chains are interlinked into a two-dimensional network by O—H···N and C—H···O hydrogen bonds involving the water molecule, which lies on a twofold rotation axis.

Comment

In our ongoing studies of triazole compounds, we have synthesized the title compound, (I). An X-ray crystallographic analysis was undertaken to establish the structure.



(I)

The bond lengths and angles in (I) (Fig. 1 and Table 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those in 1-(4-methoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one, (II) (Wan *et al.*, 2005). In contrast to the planar configuration of (II), the molecule of (I) is non-planar. The two aromatic rings are almost perpendicular to one another, with a dihedral angle of 87.12 (10)°. There is an intramolecular hydrogen bond, C1—H1···O1, forming a five-membered ring. Glide-related molecules are linked into chains along the *c* axis by intermolecular C11—H11···N3^{iii} interactions (for symmetry code, see Table 2). The water molecules, which lie

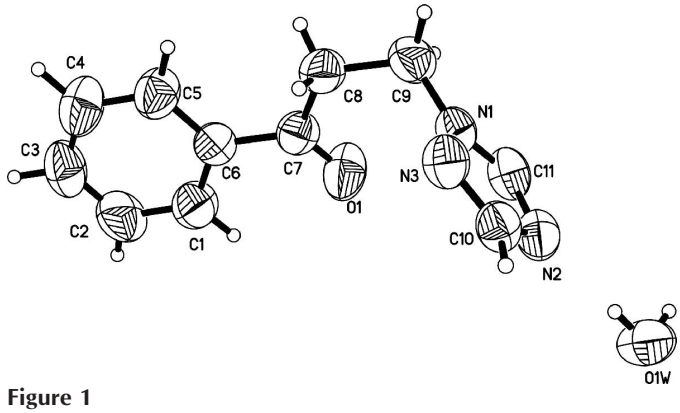


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

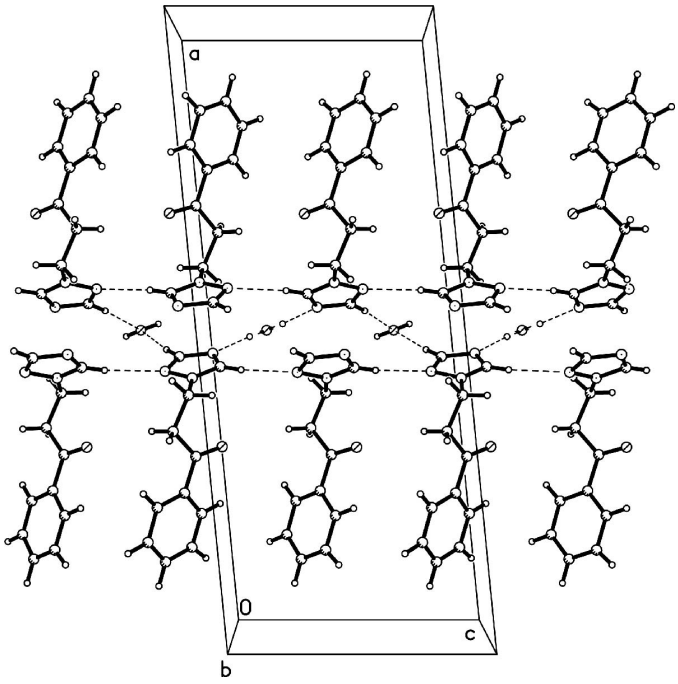


Figure 2
A view of (I) down the *b* axis. Hydrogen bonds are indicated by dashed lines.

on twofold rotation axes, act as both donors and acceptors, connecting the chains into a two-dimensional network (Fig. 2). The packing is further stabilized by π–π interactions involving the triazole ring; the triazole rings at (x, y, z) and ($1-x$, $-y$, $1-z$) are stacked with a centroid–centroid separation of 3.516 (2) Å.

Experimental

The title compound was prepared according to the literature method of Shi *et al.* (1996). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate-petroleum ether (1:1 *v*/*v*) solution over a period of two weeks.

Crystal data

$C_{11}H_{11}N_3O\cdot0.5H_2O$
M_r = 210.24
Monoclinic, $C2/c$
a = 25.429 (9) Å
b = 8.209 (5) Å
c = 10.502 (6) Å
β = 95.595 (9)°
V = 2181.9 (19) Å^3
Z = 8
D_x = 1.280 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2225 reflections
θ = 2.6–25.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.44 × 0.25 × 0.09 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.962, T_{max} = 0.992
5789 measured reflections
2141 independent reflections
1723 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.1°
$h = -31 \rightarrow 17$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.05
2141 reflections
189 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.7904P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—C11	1.320 (2)	C10—N3	1.309 (2)
N1—N3	1.3557 (19)	C10—N2	1.348 (2)
N1—C9	1.457 (2)	C7—O1	1.213 (2)
C11—N2	1.317 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···N2^{i}	0.89 (3)	2.03 (3)	2.920 (2)	176 (3)
C1—H1···O1	0.94 (2)	2.44 (3)	2.776 (3)	101 (2)
C10—H10···O1W^{ii}	0.95 (2)	2.42 (2)	3.364 (3)	173 (2)
C11—H11···N3^{iii}	0.91 (2)	2.54 (2)	3.442 (3)	170 (2)

Symmetry codes: (i) $1-x, y, \frac{3}{2}-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, -y, \frac{1}{2}+z$.

All H atoms were located in difference Fourier maps and refined isotropically. The O—H distance is 0.88 (2) Å and C—H distances lie in the range 0.92 (3)–0.98 (2) Å.

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

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