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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(C-C) = 0.002$ Å
 R factor = 0.041
 wR factor = 0.116
Data-to-parameter ratio = 12.8

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

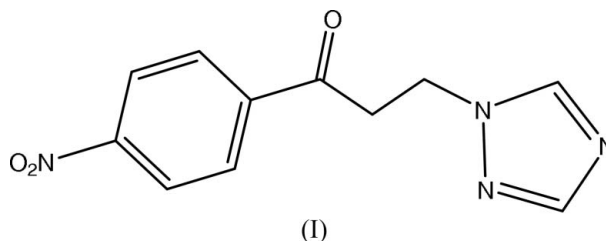
1-(4-Nitrophenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one

In the title molecule, $C_{11}H_{10}N_4O_3$, the dihedral angle between the benzene and triazole rings is $60.4(1)^\circ$. Weak intermolecular $C-H \cdots O$ hydrogen bonds and van der Waals forces stabilize the crystal packing.

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Comment

In our ongoing studies of triazole compounds, the title compound, (I), was obtained by the reaction of triazole and 3-(dimethylamino)-1-(4-nitrophenyl)propan-1-one hydrochloride. An X-ray crystallographic analysis was undertaken to establish its structure.



The bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those in related compounds (Wan, Li, Li, Li *et al.*, 2005; Wan, Li, Li, Wang *et al.*, 2005). The molecule of (I) is non-planar; the benzene and triazole rings make a dihedral angle of $60.4(1)^\circ$. In the crystal structure, weak intermolecular $C-H \cdots O$ hydrogen bonds (Table 2) link the molecules into ribbons. The packing (Table 2) is further stabilized by van der Waals forces.

Experimental

To a solution of 3-(dimethylamino)-1-(4-nitrophenyl)propan-1-one hydrochloride (18 g, 0.07 mol) in water (20 ml) was added triazole (5.5 g, 0.08 mol). The mixture was heated under reflux for 5 h, yielding a copious precipitate. Colourless single crystals suitable for

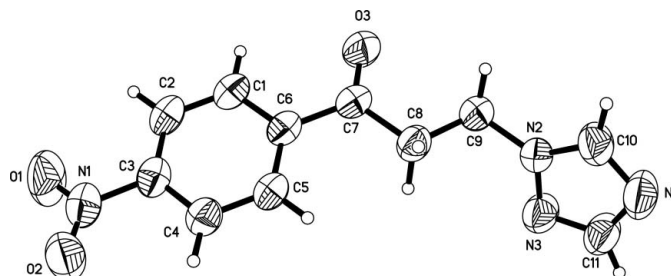


Figure 1
View of (I), showing the atom numbering scheme and 50% probability displacement ellipsoids.

an X-ray diffraction study were obtained by slow evaporation of an ethyl acetate-petroleum ether solution (2:1 v/v) over a period of 10 d.

Crystal data

$C_{11}H_{10}N_4O_3$
 $M_r = 246.23$
 Monoclinic, $P2_1/c$
 $a = 9.8529$ (7) Å
 $b = 5.4011$ (4) Å
 $c = 21.9132$ (14) Å
 $\beta = 103.233$ (3)°
 $V = 1135.18$ (14) Å³
 $Z = 4$

$D_x = 1.441$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2976 reflections
 $\theta = 2.5$ – 26.0°
 $\mu = 0.11$ mm⁻¹
 $T = 294$ (2) K
 Plate, colourless
 $0.49 \times 0.35 \times 0.11$ mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.943$, $T_{\max} = 0.984$
 6034 measured reflections

2231 independent reflections
 1956 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -11 \rightarrow 12$
 $k = -6 \rightarrow 6$
 $l = -22 \rightarrow 27$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.116$
 $S = 1.03$
 2231 reflections
 174 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 0.1874P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.030 (4)

Table 1

Selected geometric parameters (Å, °).

O3–C7	1.2077 (17)	N2–C9	1.4568 (17)
N1–C3	1.471 (2)	N3–C11	1.3104 (19)
N2–C10	1.3153 (18)	N4–C10	1.316 (2)
N2–N3	1.3499 (17)	N4–C11	1.334 (2)
C10–N2–N3	108.93 (12)	C6–C7–C8	119.03 (12)
C10–N2–C9	129.78 (13)	C9–C8–C7	110.85 (11)
C11–N3–N2	102.09 (12)	N2–C9–C8	112.69 (11)
C10–N4–C11	101.48 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C2–H2A \cdots O1 ⁱ	0.93	2.57	3.469 (2)	163
C11–H11A \cdots O2 ⁱⁱ	0.93	2.57	3.435 (2)	154

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

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve

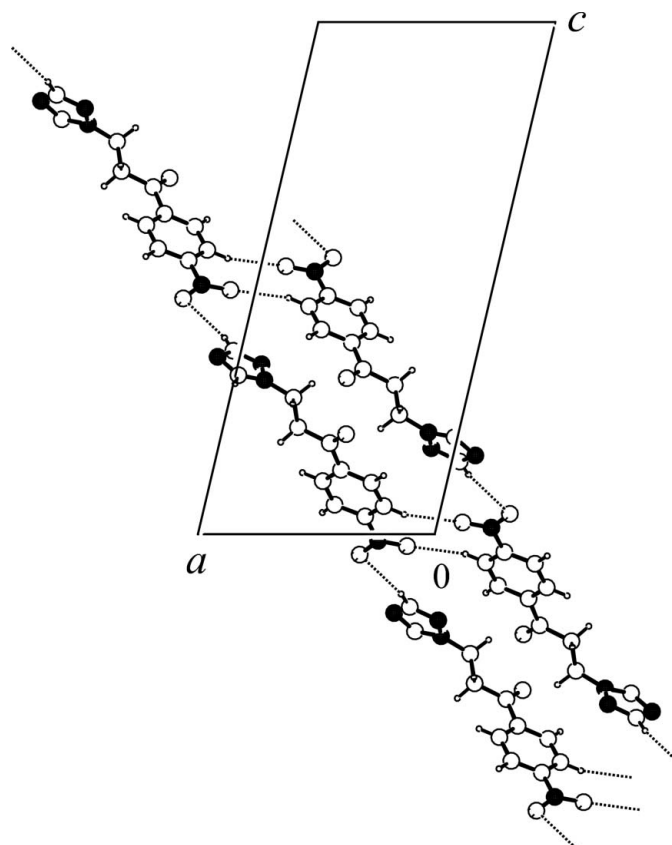


Figure 2

The crystal packing, viewed down the b axis. The intermolecular C–H \cdots O hydrogen bonds are indicated by dotted lines.

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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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, S1–19.
 Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.
 Siemens (1996). *SMART and SAINT*. Siemens Analytical X-Ray Systems, Inc., Madison, Wisconsin, USA.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Wan, J., Li, C.-L., Li, X.-M., Li, Y., Zhang, S.-S., Xu, H. & Ouyang, P.-K. (2005). *Acta Cryst.* **E61**, o1997–o1998.
 Wan, J., Li, C.-L., Li, X.-M., Wang S.-Y. & Zhang, S.-S. (2005). *Acta Cryst.* **E61**, o2391–o2392.