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3-(1*H*-Benzotriazol-1-yl)-1-(3-chlorophenyl)-propan-1-one

Wu-Lan Zeng,[a] Sai Bi,[b] Na-Na Tian[b] and Jun Wan[b]*

[a]Department of Chemistry and Chemical Engineering, Weifang University, 261061 Weifang, Shandong, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.111
Data-to-parameter ratio = 14.0

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

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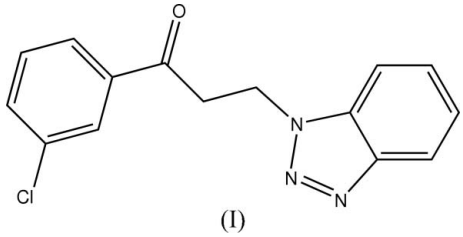
In the title compound, $C_{15}H_{12}ClN_3O$, the molecules are linked into centrosymmetric dimers by C—H···O intermolecular hydrogen bonds. The molecular packing is further stabilized by π–π interactions.

Comment

1*H*-Benzotriazole and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumour and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our ongoing studies on new benzotriazole compounds with higher bioactivity.



(I)

The non-H atoms in (I) are essentially coplanar, with a dihedral angle of 0.81 (8)° between the least-squares planes of the benzene ring and of the benzotriazole ring system.

The molecules are linked into dimers by C15—H15*A*···O3^{i} [symmetry code: (i) 1 − *x*, 1 − *y*, 1 − *z*] intermolecular hydrogen bonds (Table 1 and Fig. 2). The packing is further stabilized by π–π interactions, with a *Cg*1···*Cg*2^{ii} [symmetry code: (ii) 1 + *x*, 1 + *y*, *z*] distance of 3.759 (1) Å (*Cg*1 and *Cg*2 denote the centroids of the C1–C6 and C10–C15 rings, respectively).

Experimental

To a solution of 1-(3-chlorophenyl)-3-(dimethylamino)propan-1-one (10.58 g, 0.05 mol) in water (25 ml) was added benzotriazole (7.1 g, 0.06 mol). The mixture was heated under reflux for 5 h, yielding a copious precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane–cyclohexane (1:2 *v*/*v*) solution over a period of 6 d.

Crystal data

$C_{15}H_{12}ClN_3O$
M_r = 285.73
Triclinic, $P\overline{1}$
a = 7.4919 (9) Å
b = 7.9858 (10) Å
c = 11.4486 (14) Å
α = 92.948 (2)°
β = 96.711 (2)°
γ = 102.841 (2)°
V = 661.13 (14) Å^3
Z = 2
D_x = 1.435 Mg m^{-3}
Mo *Kα* radiation
μ = 0.29 mm^{-1}
T = 293 (2) K
Needle, colourless
0.46 × 0.17 × 0.10 mm

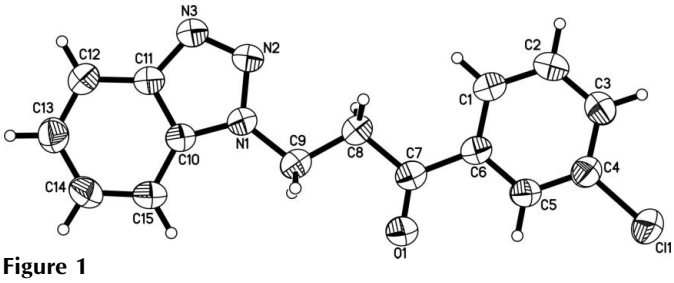


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.879, T_{max} = 0.972
3726 measured reflections
2526 independent reflections
2102 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.05
2526 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.1689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···O1^{i}	0.93	2.57	3.454 (2)	158

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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

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).

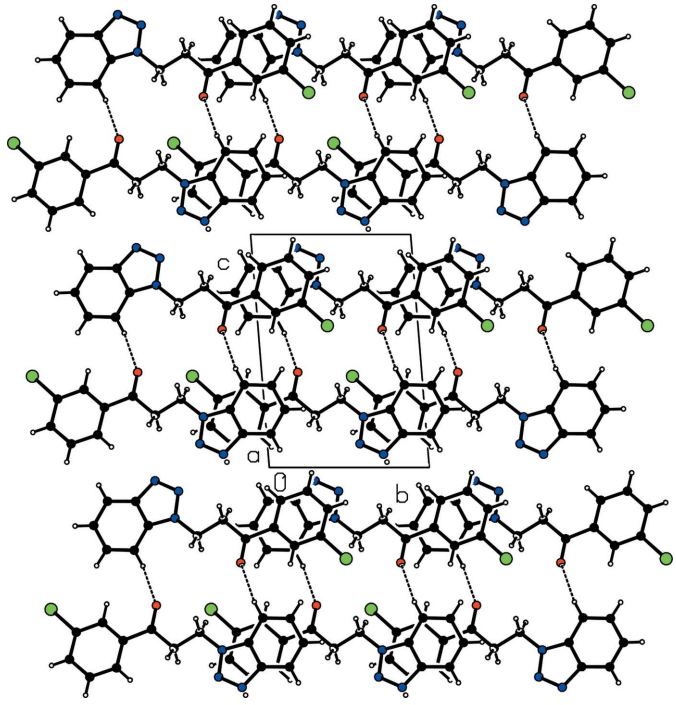


Figure 2
Packing diagram of (I), showing the intermolecular hydrogen bonds (dashed lines), viewed down the *a* axis.

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