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1-[1-(4-Nitrophenyl)-1*H*-tetrazol-5-yl]-1*H*-1,2,3-benzotriazole

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.170
Data-to-parameter ratio = 13.0

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

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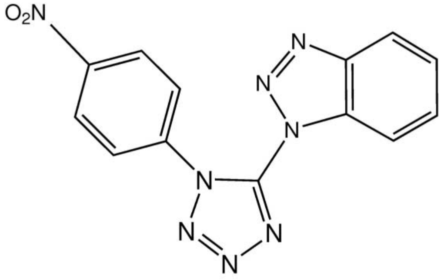
In the title compound, $C_{13}H_8N_8O_2$, the benzotriazole group forms a dihedral angle of 17.56 (12)° with the tetrazole ring and conjugation exists between them. The nitrobenzene group lies perpendicular to the tetrazole ring and there is no conjugation.

Comment

Tetrazoles find wide application in the synthesis of medicinal products such as antihypertensive agents (Wexler *et al.*, 1996; Schmidt & Schieffer, 2003; Satyanarayana *et al.*, 2006), resolvents (Bekhit *et al.*, 2004), anaesthetics (Rajasekaran & Thampi, 2004) and antifungal agents (Upadhayaya *et al.*, 2004). The title compound, (I), is a new tetrazole derivative, which is a prospective compound for preparation of new medicinal products.



(I)

Each of the four distinct rings in the molecule of (I) (Fig. 1) is essentially planar, with mean deviations of the ring atoms from their least-squares planes of 0.0030 (16), 0.0011 (13), 0.0047 (12) and 0.0038 (17) Å for the benzene ring of the nitrobenzene group (C6–C11), the tetrazole ring (N1–N4/C5), the triazole ring (N13–N15/C16/C17) and the benzene ring (C16–C21) of the benzotriazole group, respectively. The dihedral angle between the latter two rings is 0.86 (13)°. The triazole and tetrazole rings are rotated with respect to each other around the C5—N13 bond to give a dihedral angle of 17.56 (12)°. The nitrobenzene ring lies essentially perpendicular to the tetrazole ring, forming a dihedral angle of 90.00 (7)°. This suggests that conjugation exists between the tetrazole and benzotriazole rings, but not between the nitrobenzene and tetrazole rings. This observation is supported by significant shortening of the C5—N13 bond [1.385 (2) Å] compared with the N1—C6 bond [1.438 (2) Å]. The geometry of the tetrazole ring is typical of other 1- and 1,5-substituted tetrazoles in the Cambridge Structural Database (Version 5.27; Allen, 2002). Between molecules, C—H···N and C—H···O interactions are observed (Fig. 2 and Table 1).

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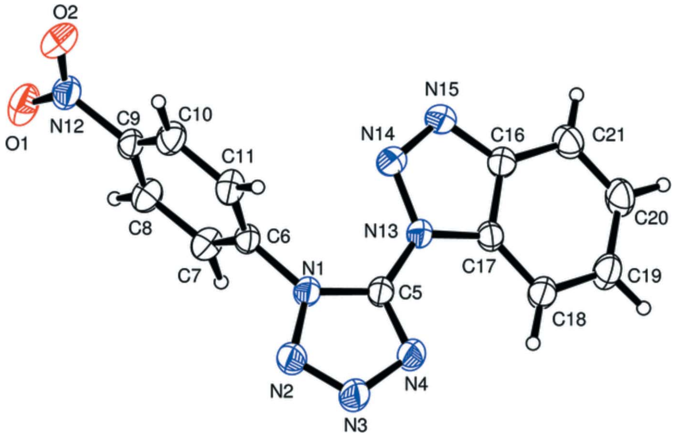

Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

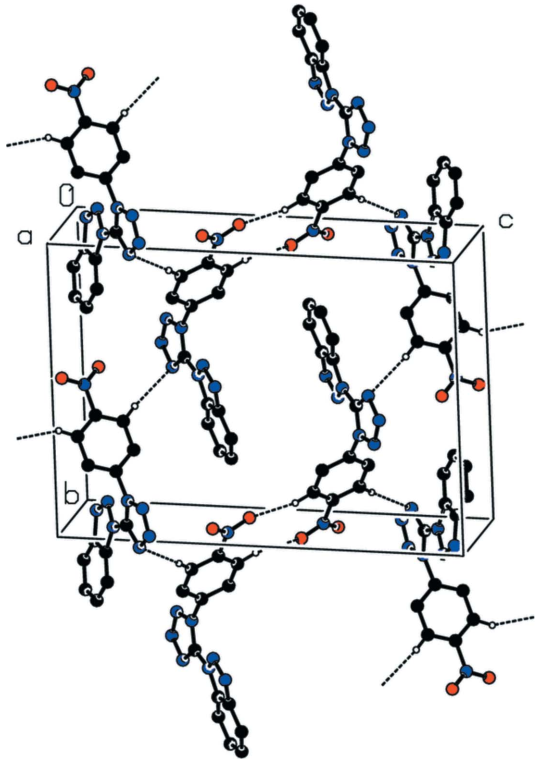

Figure 2
C—H···O and C—H···N interactions (dashed lines) in (I). H atoms not participating in these interactions have been omitted.

Experimental

Benzotriazole (0.24 g, 2 mmol) and NaOH (0.12 g, 3 mmol) were added to a solution of 5-methylsulfinyl-1-(4-nitrophenyl)tetrazole (0.5 g, 2 mmol) in acetonitrile (10 ml). The reaction mixture was stirred for 1.5 h at room temperature. Ice–water (50 ml) was then added to the mixture and the resulting precipitate of (I) was filtered off, dried in air and recrystallized from a mixture of ethanol–DMF (*v*/*v* 3:1) (yield 0.48 g, 80%; m.p. 498–499 K).

Crystal data

$C_{13}H_8N_8O_2$
$M_r = 308.27$
Monoclinic, $P2_1/c$
$a = 5.0841\ (17)$ Å
$b = 14.024\ (4)$ Å
$c = 18.836\ (6)$ Å
$\beta = 92.14\ (3)^\circ$
$V = 1342.1\ (7)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 292\ (2)$ K
$0.36 \times 0.24 \times 0.16$ mm

Data collection

Nicolet R3m diffractometer
Absorption correction: none
3457 measured reflections
3113 independent reflections
1933 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.068$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.170$
$S = 1.05$
3113 reflections
240 parameters
All H-atom parameters refined
$\Delta\rho_{\rm max} = 0.17$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1$^{\rm i}$	0.97 (2)	2.51 (2)	3.401 (3)	153.5 (19)
C10—H10···N4$^{\rm ii}$	0.94 (2)	2.60 (3)	3.535 (3)	172 (2)

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

H atoms were located in a difference Fourier map and refined freely with isotropic displacement parameters. The refined C—H bond lengths are in the range 0.89 (2)–1.01 (3) Å.

Data collection: *R3m Software* (Nicolet, 1980); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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