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5-(4-Methyl-3-nitrophenyl)-1*H*-tetrazole

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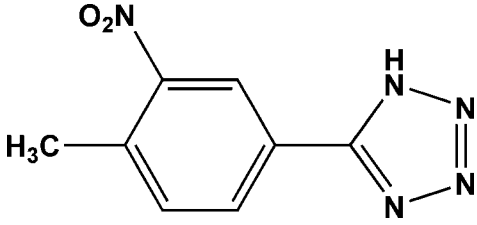
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.076; wR factor = 0.191; data-to-parameter ratio = 14.9.

In the title compound, $C_8H_7N_5O_2$, the benzene ring makes a dihedral angle of 38.27 (11)° with the tetrazole ring. The crystal structure is stabilized by N—H···N hydrogen bonds, forming an infinite one-dimensional chain parallel to the *a* axis.

Related literature

For the use of tetrazole derivatives in coordination chemisty, see: Arp *et al.* (2000); Hu *et al.* (2007); Wang *et al.* (2005); Xiong *et al.* (2002).



Experimental

Crystal data

$C_8H_7N_5O_2$
M_r = 205.19
Monoclinic, $P2_1/c$
a = 4.9642 (10) Å
b = 16.982 (3) Å
c = 10.804 (2) Å
β = 100.71 (3)°
V = 894.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.971, T_{max} = 0.977
7013 measured reflections
2039 independent reflections
1330 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.190
S = 1.08
2039 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4^{i}	0.86	2.01	2.832 (3)	160

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2361).

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5-(4-Methyl-3-nitrophenyl)-1*H*-tetrazole

Wei Dai and Da-Wei Fu

S1. Comment

In the past five years, our work have been focused on the chemistry of tetrazole derivatives because of their multiple coordination modes as ligands to metal ions and for the construction of novel metal-organic frameworks (Wang *et al.*, 2005; Xiong *et al.*, 2002). We report here the crystal structure of the title compound, 5-(4-methyl-3-nitrophenyl)-2*H*-tetrazole, (Fig.1).

The benzene ring makes a dihedral angle of 38.27 (0.11) ° with the tetrazole ring owing to the C–C bond bridge which force the two rings to be twisted from each other. The bond distances and bond angles of the tetrazole rings are in the usual ranges (Wang *et al.*, 2005; Arp *et al.* , 2000; Hu *et al.*, 2007). The crystal packing is stabilized by N—H···N hydrogen bonds to form an infinite one-dimensional chain parallel to the *a* axis. (Table 1, Fig. 2).

S2. Experimental

5-(4-methyl-3-nitrophenyl)-2*H*-tetrazole (3 mmol) was dissolved in ethanol (20 ml) and evaporated in the air affording colorless block crystals of this compound suitable for X-ray analysis were obtained.

S3. Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding with C–H = 0.9 Å (aromatic),0.96 Å(methyl) and N–H = 0.86 Å with U_{iso}(H) =1.2Ueq(C or N).

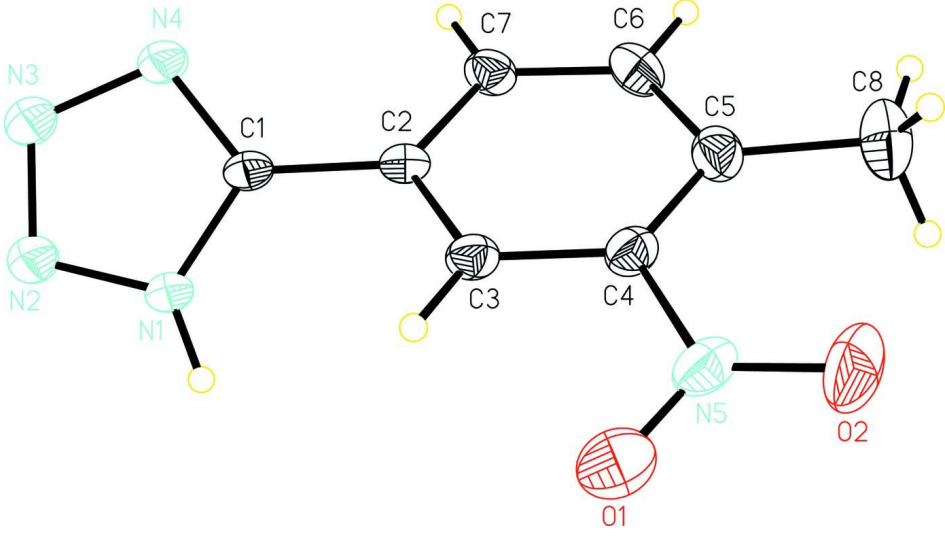

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

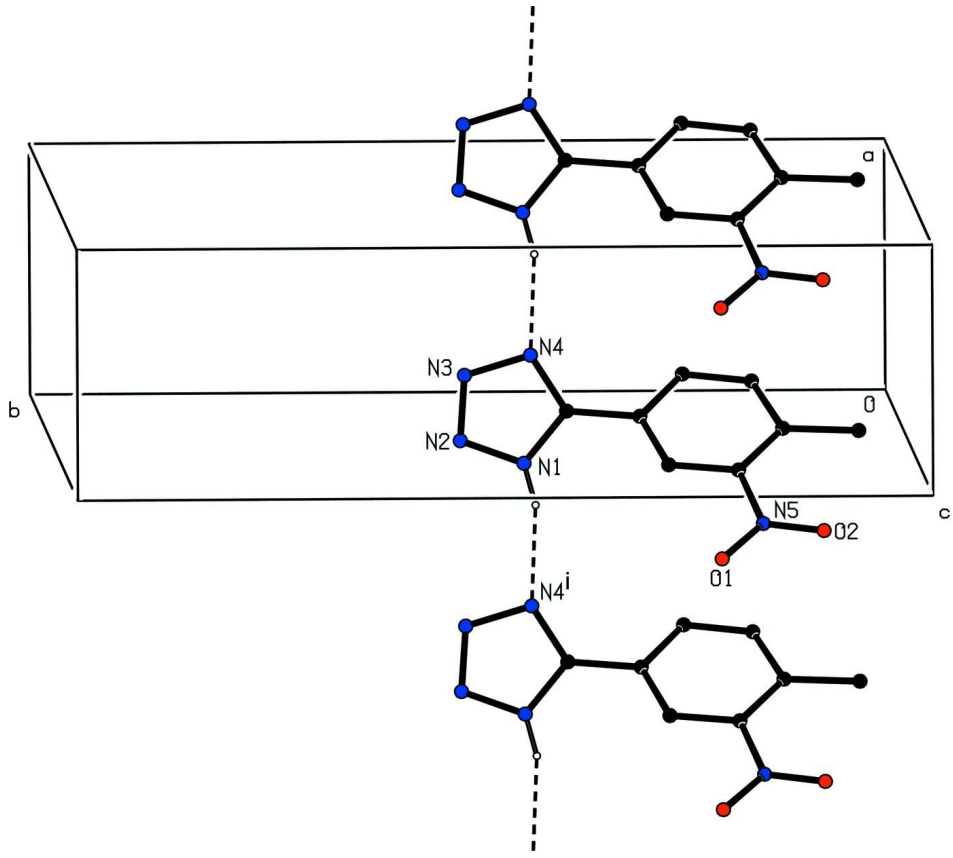

Figure 2

Partial packing of the title compound showing the one dimensionnal hydrogen bondings network. Hydrogen atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity. [Symmetry code : (i) x-1, y, z]

5-(4-Methyl-3-nitrophenyl)-1*H*-tetrazole

Crystal data

$C_8H_7N_5O_2$
$M_r = 205.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.9642\ (10)$ Å
$b = 16.982\ (3)$ Å
$c = 10.804\ (2)$ Å
$\beta = 100.71\ (3)°$
$V = 894.9\ (3)$ Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.523$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2043 reflections
$\theta = 3.1–27.5°$
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Block, colorless
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.971$, $T_{max} = 0.977$
7013 measured reflections
2039 independent reflections
1330 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$

θ_{max} = 27.5°, θ_{min} = 3.1°
h = −6→6
k = −22→21
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.190
S = 1.08
2039 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0844P)^2 + 0.0553P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.037 (7)

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 $F^2 > \sigma(F^2)$ 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}
N1	0.0809 (4)	0.47072 (13)	0.8636 (2)	0.0355 (6)
H1A	−0.0824	0.4579	0.8719	0.043*
N4	0.5077 (4)	0.46190 (13)	0.8535 (2)	0.0375 (6)
C1	0.2914 (5)	0.42106 (15)	0.8715 (2)	0.0300 (6)
C2	0.2791 (5)	0.33663 (15)	0.8959 (2)	0.0316 (6)
N2	0.1626 (5)	0.54380 (12)	0.8406 (2)	0.0429 (6)
N3	0.4204 (5)	0.53814 (13)	0.8340 (2)	0.0445 (6)
C3	0.1202 (5)	0.30784 (15)	0.9784 (2)	0.0346 (6)
H3A	0.0240	0.3423	1.0211	0.041*
C4	0.1057 (5)	0.22713 (16)	0.9969 (2)	0.0360 (7)
C7	0.4202 (6)	0.28333 (16)	0.8331 (3)	0.0380 (6)
H7A	0.5288	0.3016	0.7777	0.046*
C6	0.3991 (6)	0.20365 (16)	0.8530 (3)	0.0448 (7)
H6A	0.4927	0.1694	0.8089	0.054*
C5	0.2449 (6)	0.17202 (15)	0.9358 (3)	0.0423 (7)
O1	−0.1907 (5)	0.25440 (14)	1.1326 (2)	0.0687 (8)
O2	−0.0896 (5)	0.13387 (15)	1.1108 (2)	0.0781 (9)
N5	−0.0701 (5)	0.20355 (16)	1.0866 (2)	0.0468 (7)
C8	0.2416 (8)	0.08409 (18)	0.9527 (4)	0.0681 (10)
H8A	0.3551	0.0599	0.9006	0.102*
H8B	0.0571	0.0650	0.9289	0.102*

H8C	0.3103	0.0713	1.0393	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0248 (12)	0.0353 (12)	0.0489 (14)	−0.0016 (9)	0.0130 (9)	0.0005 (9)
N4	0.0280 (12)	0.0381 (13)	0.0489 (15)	−0.0015 (9)	0.0138 (9)	0.0055 (10)
C1	0.0237 (13)	0.0375 (14)	0.0308 (13)	−0.0009 (10)	0.0101 (9)	−0.0005 (10)
C2	0.0231 (13)	0.0376 (14)	0.0350 (15)	0.0014 (10)	0.0076 (10)	−0.0001 (10)
N2	0.0352 (13)	0.0384 (14)	0.0569 (16)	−0.0006 (10)	0.0135 (11)	0.0049 (11)
N3	0.0366 (14)	0.0415 (14)	0.0587 (16)	−0.0041 (10)	0.0172 (11)	0.0038 (11)
C3	0.0295 (15)	0.0390 (15)	0.0374 (16)	0.0000 (11)	0.0120 (11)	−0.0006 (11)
C4	0.0320 (15)	0.0399 (15)	0.0363 (15)	−0.0035 (11)	0.0065 (11)	0.0057 (11)
C7	0.0349 (15)	0.0411 (15)	0.0406 (16)	0.0059 (11)	0.0141 (12)	−0.0002 (12)
C6	0.0464 (18)	0.0422 (17)	0.0466 (18)	0.0123 (13)	0.0106 (13)	−0.0044 (12)
C5	0.0426 (17)	0.0371 (16)	0.0442 (17)	0.0017 (12)	0.0005 (13)	0.0024 (12)
O1	0.0701 (17)	0.0762 (17)	0.0721 (17)	−0.0033 (13)	0.0451 (13)	0.0098 (13)
O2	0.096 (2)	0.0572 (16)	0.087 (2)	−0.0154 (12)	0.0304 (16)	0.0263 (13)
N5	0.0377 (15)	0.0574 (17)	0.0444 (15)	−0.0108 (11)	0.0053 (11)	0.0132 (12)
C8	0.091 (3)	0.0377 (18)	0.074 (3)	−0.0006 (17)	0.011 (2)	0.0031 (16)

Geometric parameters (Å, º)

N1—C1	1.333 (3)	C4—N5	1.475 (3)
N1—N2	1.343 (3)	C7—C6	1.377 (4)
N1—H1A	0.8600	C7—H7A	0.9300
N4—C1	1.323 (3)	C6—C5	1.388 (4)
N4—N3	1.369 (3)	C6—H6A	0.9300
C1—C2	1.461 (3)	C5—C8	1.505 (4)
C2—C3	1.385 (3)	O1—N5	1.209 (3)
C2—C7	1.395 (3)	O2—N5	1.220 (3)
N2—N3	1.299 (3)	C8—H8A	0.9600
C3—C4	1.389 (4)	C8—H8B	0.9600
C3—H3A	0.9300	C8—H8C	0.9600
C4—C5	1.400 (4)		
C1—N1—N2	109.7 (2)	C6—C7—C2	120.1 (2)
C1—N1—H1A	125.2	C6—C7—H7A	119.9
N2—N1—H1A	125.2	C2—C7—H7A	119.9
C1—N4—N3	106.0 (2)	C7—C6—C5	123.2 (3)
N4—C1—N1	107.9 (2)	C7—C6—H6A	118.4
N4—C1—C2	127.1 (2)	C5—C6—H6A	118.4
N1—C1—C2	125.0 (2)	C6—C5—C4	115.1 (2)
C3—C2—C7	118.8 (2)	C6—C5—C8	118.8 (3)
C3—C2—C1	120.7 (2)	C4—C5—C8	126.0 (3)
C7—C2—C1	120.5 (2)	O1—N5—O2	122.7 (3)
N3—N2—N1	106.0 (2)	O1—N5—C4	118.4 (2)
N2—N3—N4	110.4 (2)	O2—N5—C4	119.0 (3)

C2—C3—C4	119.5 (2)	C5—C8—H8A	109.5
C2—C3—H3A	120.3	C5—C8—H8B	109.5
C4—C3—H3A	120.3	H8A—C8—H8B	109.5
C5—C4—C3	123.3 (2)	C5—C8—H8C	109.5
C5—C4—N5	122.2 (3)	H8A—C8—H8C	109.5
C3—C4—N5	114.5 (2)	H8B—C8—H8C	109.5
N3—N4—C1—N1	−0.1 (3)	C2—C3—C4—N5	−179.9 (2)
N3—N4—C1—C2	179.8 (2)	C3—C2—C7—C6	0.4 (4)
N2—N1—C1—N4	−0.2 (3)	C1—C2—C7—C6	−177.5 (2)
N2—N1—C1—C2	179.9 (2)	C2—C7—C6—C5	−1.1 (4)
N4—C1—C2—C3	142.9 (3)	C7—C6—C5—C4	1.2 (4)
N1—C1—C2—C3	−37.2 (4)	C7—C6—C5—C8	−178.5 (3)
N4—C1—C2—C7	−39.2 (4)	C3—C4—C5—C6	−0.6 (4)
N1—C1—C2—C7	140.7 (3)	N5—C4—C5—C6	179.2 (2)
C1—N1—N2—N3	0.4 (3)	C3—C4—C5—C8	179.1 (3)
N1—N2—N3—N4	−0.5 (3)	N5—C4—C5—C8	−1.1 (4)
C1—N4—N3—N2	0.4 (3)	C5—C4—N5—O1	−177.7 (3)
C7—C2—C3—C4	0.1 (4)	C3—C4—N5—O1	2.2 (4)
C1—C2—C3—C4	178.1 (2)	C5—C4—N5—O2	1.9 (4)
C2—C3—C4—C5	0.0 (4)	C3—C4—N5—O2	−178.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N4^{i}	0.86	2.01	2.832 (3)	160

Symmetry code: (i) *x*−1, *y*, *z*.