

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

5-[4-(1*H*-Imidazol-1-yl)phenyl]-1*H*-tetrazoleShao-Wei Tong,^a Wen-Dong Song,^{b*} Shi-Jie Li,^c
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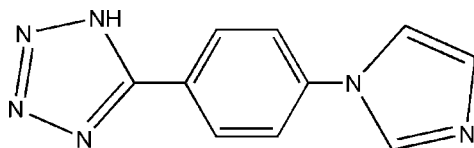
Received 21 March 2012; accepted 29 March 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.039; wR factor = 0.120; data-to-parameter ratio = 9.8.

In the title compound, $\text{C}_{10}\text{H}_8\text{N}_6$, the tetrazole and benzene rings are close to being coplanar [dihedral angle = 9.90 (16°)], but the imidazole ring is rotated 37.18 (09°) out of the benzene plane. In the crystal, molecules are connected through tetrazole–imidazole $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds, giving rise to zigzag chains, which extend along [010].

Related literature

For our previous work based on the imidazole derivatives as ligands, see: Li *et al.* (2010); Tong *et al.* (2011); Tong *et al.*, (2012). For related structures, see: Huang *et al.* (2009); Cheng (2011).



Experimental

Crystal data

$\text{C}_{10}\text{H}_8\text{N}_6$	$V = 472.6$ (3) Å ³
$M_r = 212.22$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 3.7219$ (12) Å	$\mu = 0.10$ mm ⁻¹
$b = 16.429$ (5) Å	$T = 296$ K
$c = 7.791$ (2) Å	$0.30 \times 0.20 \times 0.15$ mm
$\beta = 97.167$ (6)°	

Data collection

Bruker SMART CCD area-detector diffractometer	3477 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	1421 independent reflections
$T_{\min} = 0.971$, $T_{\max} = 0.985$	1239 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$	1 restraint
$wR(F^2) = 0.120$	H-atom parameters constrained
$S = 1.35$	$\Delta\rho_{\text{max}} = 0.25$ e Å ⁻³
1421 reflections	$\Delta\rho_{\text{min}} = -0.31$ e Å ⁻³
145 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3}\cdots\text{N2}^i$	0.86	1.93	2.751 (4)	158

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

We acknowledge the Public Science and Technology Research Funds Projects of Ocean (grant No. 2000905021), the Guangdong Oceanic Fisheries Technology Promotion Project [grant No. A2009003-018(c)], the Guangdong Chinese Academy of Science Comprehensive Strategic Cooperation Project (grant No. 2009B091300121) and the Guangdong Province Key Project in the Field of Social Development [grant No. A2009011-007(c)].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2194).

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supporting information

Acta Cryst. (2012). E68, o1274 [doi:10.1107/S1600536812013670]

5-[4-(1*H*-Imidazol-1-yl)phenyl]-1*H*-tetrazole

Shao-Wei Tong, Wen-Dong Song, Shi-Jie Li, Dong-Liang Miao and Jing-Bo An

S1. Comment

The imidazole derivatives can be used to synthesize various types of metal complexes because they contain available *N*-donor sites for coordination. Our research group has shown great interest in metal-organic complexes with imidazole derivatives, e.g. 2-propylimidazole-4,5-dicarboxylic acid (Tong *et al.*, 2011; Li *et al.*, 2010) and 5-[4-imidazol-1-yl]phenyl]tetrazole (1-tetrazole-4-imidazolebenzene) (Tong *et al.*, 2012). In this paper, we report the crystal structure of this ligand from crystals obtained under hydrothermal conditions. As illustrated in Fig. 1, the tetrazole and benzene rings are close to coplanar [dihedral angle, 9.90 (16)°] but the imidazole ring is rotated 37.18 (19)° out of the benzene plane. The molecules are connected into one-dimensional zigzag chains through tetrazole N—H⋯N_{imidazole} hydrogen bonds (Table 1, Fig. 2). For the structures of complexes with this ligand, see Huang *et al.* (2009) and Cheng (2011).

S2. Experimental

5-[4-imidazol-1-yl]phenyl]tetrazole (0.2 mmol, 0.043 g) in 12 ml of *N,N*-dimethylformamide was sealed in an autoclave equipped with a Teflon liner (25 ml) and then heated at 413 K for 3 days. Crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

S3. Refinement

The imidazolyl and phenyl H-atoms and the tetrazole N H-atom were located in a difference-Fourier but were refined as riding with C—H = 0.93 Å or N—H = 0.86 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

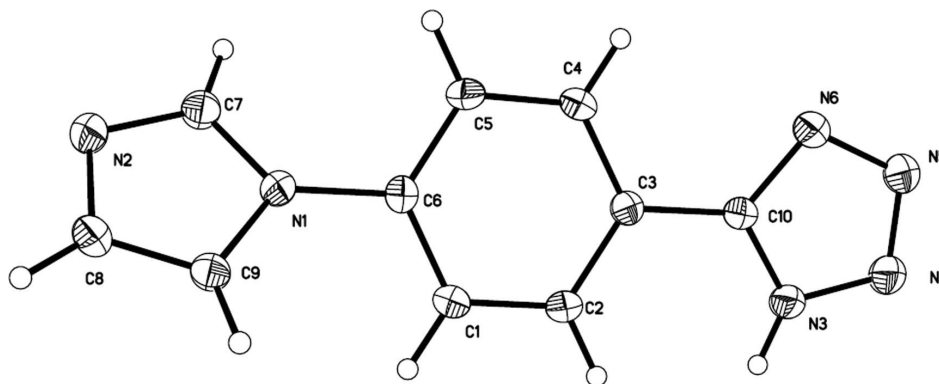


Figure 1

Molecular conformation and atom numbering scheme for the title compound, showing 30% probability displacement ellipsoids.

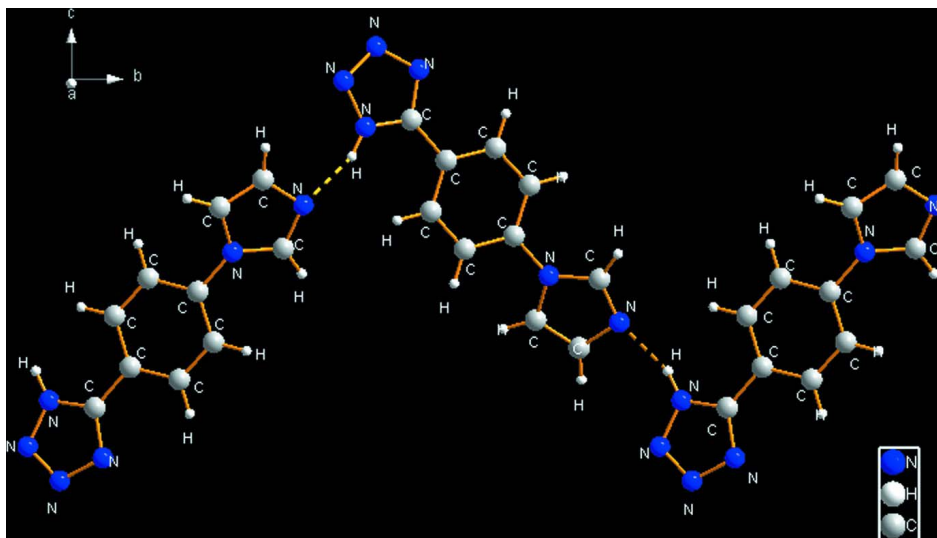


Figure 2

The one-dimensional chain structure extending along [010], with hydrogen bonds shown as dashed lines.

5-[4-(1*H*-Imidazol-1-yl)phenyl]-1*H*-tetrazole

Crystal data

$C_{10}H_8N_6$

$M_r = 212.22$

Monoclinic, $P2_1$

Hall symbol: P 2yb

$a = 3.7219$ (12) Å

$b = 16.429$ (5) Å

$c = 7.791$ (2) Å

$\beta = 97.167$ (6)°

$V = 472.6$ (3) Å³

$Z = 2$

$F(000) = 220$

$D_x = 1.491$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1003 reflections

$\theta = 2.6$ – 22.3 °

$\mu = 0.10$ mm⁻¹

$T = 296$ K

Block, colorless

$0.30 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.971$, $T_{\max} = 0.985$

3477 measured reflections

1421 independent reflections

1239 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.5$ °

$h = -4 \rightarrow 4$

$k = -19 \rightarrow 18$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.120$

$S = 1.35$

1421 reflections

145 parameters

1 restraint

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

$$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.001P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.25 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.31 \text{ e } \text{Å}^{-3}$$

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 (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.9106 (8)	0.45885 (16)	0.5643 (3)	0.0314 (7)
N2	0.9495 (8)	0.57050 (19)	0.7228 (4)	0.0388 (8)
N3	0.3005 (9)	0.16887 (18)	0.0321 (4)	0.0370 (8)
H3	0.2517	0.1475	0.1273	0.044*
N4	0.2320 (10)	0.13459 (19)	-0.1262 (4)	0.0451 (9)
N5	0.3436 (11)	0.1857 (2)	-0.2329 (4)	0.0487 (9)
N6	0.4867 (9)	0.2536 (2)	-0.1484 (4)	0.0422 (8)
C1	0.6945 (10)	0.3256 (2)	0.4631 (4)	0.0350 (9)
H1A	0.6956	0.3095	0.5776	0.042*
C2	0.5860 (10)	0.2723 (2)	0.3310 (4)	0.0352 (9)
H2A	0.5189	0.2195	0.3563	0.042*
C3	0.5757 (9)	0.2967 (2)	0.1594 (4)	0.0276 (8)
C4	0.6843 (9)	0.3746 (2)	0.1250 (4)	0.0326 (8)
H4A	0.6805	0.3911	0.0106	0.039*
C5	0.7988 (9)	0.4287 (2)	0.2560 (4)	0.0330 (9)
H5A	0.8719	0.4810	0.2308	0.040*
C6	0.8024 (9)	0.4037 (2)	0.4249 (4)	0.0287 (8)
C7	0.8324 (9)	0.5391 (2)	0.5711 (4)	0.0350 (9)
H7A	0.7107	0.5684	0.4796	0.042*
C8	1.1139 (10)	0.5070 (2)	0.8171 (4)	0.0359 (9)
H8A	1.2250	0.5110	0.9305	0.043*
C9	1.0919 (10)	0.4384 (2)	0.7229 (4)	0.0338 (8)
H9A	1.1812	0.3873	0.7578	0.041*
C10	0.4558 (10)	0.2411 (2)	0.0171 (4)	0.0310 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0388 (17)	0.0255 (18)	0.0297 (16)	0.0014 (13)	0.0032 (13)	0.0001 (13)
N2	0.050 (2)	0.0313 (17)	0.0346 (16)	0.0023 (15)	0.0045 (14)	-0.0022 (14)
N3	0.0485 (19)	0.0313 (18)	0.0303 (16)	-0.0028 (15)	0.0015 (14)	0.0012 (13)
N4	0.062 (2)	0.0357 (19)	0.0359 (18)	-0.0056 (17)	0.0009 (15)	-0.0041 (15)

N5	0.074 (3)	0.039 (2)	0.0330 (19)	-0.0032 (18)	0.0052 (18)	-0.0041 (16)
N6	0.059 (2)	0.0367 (18)	0.0318 (16)	-0.0055 (16)	0.0080 (15)	-0.0003 (15)
C1	0.047 (2)	0.032 (2)	0.0268 (19)	0.0006 (18)	0.0065 (16)	0.0046 (15)
C2	0.048 (2)	0.027 (2)	0.0317 (19)	-0.0044 (17)	0.0078 (16)	0.0036 (15)
C3	0.0263 (17)	0.0287 (19)	0.0279 (17)	0.0004 (15)	0.0040 (14)	-0.0004 (15)
C4	0.040 (2)	0.034 (2)	0.0249 (19)	-0.0007 (17)	0.0053 (16)	0.0049 (15)
C5	0.038 (2)	0.028 (2)	0.0338 (19)	-0.0045 (17)	0.0094 (16)	0.0049 (15)
C6	0.0290 (19)	0.0288 (19)	0.0281 (18)	0.0000 (16)	0.0027 (15)	-0.0034 (15)
C7	0.037 (2)	0.033 (2)	0.034 (2)	0.0034 (17)	0.0001 (16)	0.0018 (15)
C8	0.039 (2)	0.040 (2)	0.0278 (17)	0.0008 (18)	0.0023 (15)	0.0000 (17)
C9	0.039 (2)	0.031 (2)	0.0293 (18)	0.0042 (17)	-0.0018 (15)	0.0032 (15)
C10	0.0362 (19)	0.029 (2)	0.0281 (19)	-0.0020 (16)	0.0054 (15)	0.0017 (15)

Geometric parameters (Å, °)

N1—C7	1.353 (4)	C1—H1A	0.9300
N1—C9	1.374 (4)	C2—C3	1.392 (4)
N1—C6	1.433 (4)	C2—H2A	0.9300
N2—C7	1.313 (4)	C3—C4	1.377 (5)
N2—C8	1.376 (5)	C3—C10	1.463 (4)
N3—C10	1.332 (5)	C4—C5	1.381 (5)
N3—N4	1.351 (4)	C4—H4A	0.9300
N3—H3	0.8600	C5—C6	1.377 (4)
N4—N5	1.286 (5)	C5—H5A	0.9300
N5—N6	1.369 (5)	C7—H7A	0.9300
N6—C10	1.324 (4)	C8—C9	1.342 (5)
C1—C2	1.374 (5)	C8—H8A	0.9300
C1—C6	1.387 (5)	C9—H9A	0.9300
C7—N1—C9	106.7 (3)	C3—C4—H4A	119.2
C7—N1—C6	127.2 (3)	C5—C4—H4A	119.2
C9—N1—C6	125.9 (3)	C6—C5—C4	118.7 (3)
C7—N2—C8	105.0 (3)	C6—C5—H5A	120.7
C10—N3—N4	109.0 (3)	C4—C5—H5A	120.7
C10—N3—H3	125.5	C5—C6—C1	120.8 (3)
N4—N3—H3	125.5	C5—C6—N1	120.2 (3)
N5—N4—N3	106.2 (3)	C1—C6—N1	118.9 (3)
N4—N5—N6	111.0 (3)	N2—C7—N1	111.7 (3)
C10—N6—N5	105.4 (3)	N2—C7—H7A	124.2
C2—C1—C6	119.6 (3)	N1—C7—H7A	124.2
C2—C1—H1A	120.2	C9—C8—N2	110.6 (3)
C6—C1—H1A	120.2	C9—C8—H8A	124.7
C1—C2—C3	120.4 (3)	N2—C8—H8A	124.7
C1—C2—H2A	119.8	C8—C9—N1	106.0 (3)
C3—C2—H2A	119.8	C8—C9—H9A	127.0
C4—C3—C2	118.7 (3)	N1—C9—H9A	127.0
C4—C3—C10	120.1 (3)	N6—C10—N3	108.3 (3)
C2—C3—C10	121.1 (3)	N6—C10—C3	125.9 (3)

C3—C4—C5	121.7 (3)	N3—C10—C3	125.8 (3)
C10—N3—N4—N5	-0.2 (4)	C9—N1—C6—C1	35.1 (5)
N3—N4—N5—N6	0.2 (4)	C8—N2—C7—N1	0.5 (4)
N4—N5—N6—C10	-0.1 (5)	C9—N1—C7—N2	-0.4 (4)
C6—C1—C2—C3	-1.5 (5)	C6—N1—C7—N2	175.1 (3)
C1—C2—C3—C4	1.5 (5)	C7—N2—C8—C9	-0.5 (4)
C1—C2—C3—C10	-179.1 (3)	N2—C8—C9—N1	0.3 (4)
C2—C3—C4—C5	-0.7 (5)	C7—N1—C9—C8	0.0 (4)
C10—C3—C4—C5	179.9 (3)	C6—N1—C9—C8	-175.5 (3)
C3—C4—C5—C6	-0.2 (5)	N5—N6—C10—N3	-0.1 (4)
C4—C5—C6—C1	0.2 (5)	N5—N6—C10—C3	179.3 (3)
C4—C5—C6—N1	-178.4 (3)	N4—N3—C10—N6	0.2 (4)
C2—C1—C6—C5	0.7 (5)	N4—N3—C10—C3	-179.2 (3)
C2—C1—C6—N1	179.2 (3)	C4—C3—C10—N6	10.2 (6)
C7—N1—C6—C5	39.0 (5)	C2—C3—C10—N6	-169.2 (4)
C9—N1—C6—C5	-146.3 (3)	C4—C3—C10—N3	-170.6 (3)
C7—N1—C6—C1	-139.6 (4)	C2—C3—C10—N3	10.0 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3...N2 ⁱ	0.86	1.93	2.751 (4)	158

Symmetry code: (i) $-x+1, y-1/2, -z+1$.