organic compounds

5-[4-(1H-Imidazol-1-yl)phenyl]-1H-tetra-zole

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In the title compound, $C_{10}H_8N_6$, 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 N—H···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).
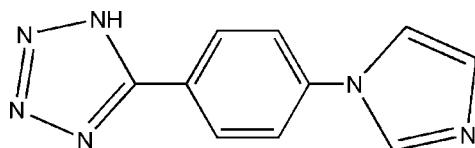
Experimental

Crystal data

$C_{10}H_8N_6$
M_r = 212.22
Monoclinic, $P2_1$
a = 3.7219 (12) Å
b = 16.429 (5) Å
c = 7.791 (2) Å
β = 97.167 (6)°

V = 472.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
$0.30 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
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_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.120
S = 1.35
1421 reflections
145 parameters

1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···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*.

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

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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$_{\text{imidazole}}$ hydrogen bonds (Table 1, Fig. 2). For the structures of complexes with this ligand, see Huang *et al.* (2009) and Cheng (2011).

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.

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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Sheldrick, 2008).
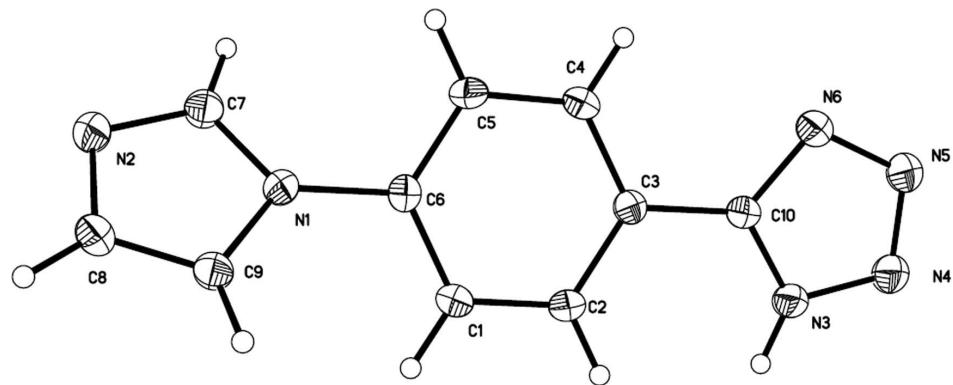
Figure 1

Molecular conformation and atom numbering scheme for the title compound, showing 30% probability displacement ellipsoids.
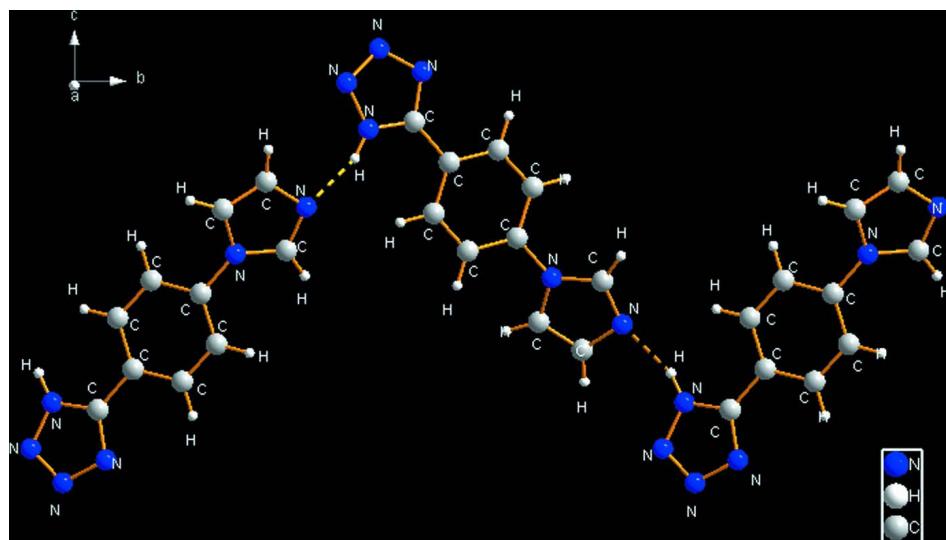
Figure 2

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

$C_{10}H_8N_6$	$F(000) = 220$
$M_r = 212.22$	$D_x = 1.491$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1003 reflections
$a = 3.7219$ (12) Å	$\theta = 2.6–22.3°$
$b = 16.429$ (5) Å	$\mu = 0.10$ mm^{-1}
$c = 7.791$ (2) Å	$T = 296$ K
$\beta = 97.167$ (6)°	Block, colorless
$V = 472.6$ (3) Å^3	$0.30 \times 0.20 \times 0.15$ mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	3477 measured reflections
Radiation source: fine-focus sealed tube	1421 independent reflections
Graphite monochromator	1239 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.038$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
	$h = -4 \rightarrow 4$
$T_{min} = 0.971$, $T_{max} = 0.985$	$k = -19 \rightarrow 18$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.120$	
$S = 1.35$	H-atom parameters constrained
1421 reflections	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.001P]$ where $P = (F_o^2 + 2F_c^2)/3$
145 parameters	
1 restraint	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.25$ e Å^{-3}
	$\Delta\rho_{min} = -0.31$ e 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)

	x	y	z	U_{iso}*/U_{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, º)

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, º)

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N2[i]	0.86	1.93	2.751 (4)	158

Symmetry code: (i) −x+1, y−1/2, −z+1.