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5-(4-Chlorophenyl)-1*H*-tetrazole

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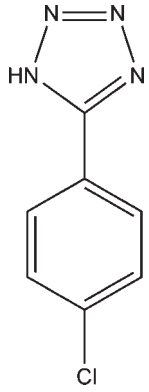
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.135; data-to-parameter ratio = 14.6.

The two independent molecules of the title compound, $C_7H_5ClN_4$, both lie on a twofold rotation axis that passes through the centroids of the five- and six-membered rings and the attached Cl C atom. One molecule is nearly planar [dihedral angle between rings = 0.22 (6)°], whereas the other is significantly twisted [dihedral angle = 17.38 (6)°]. In the crystal, adjacent molecules are linked by N—H···N hydrogen bonds into a chain structure.

Related literature

For the synthesis, see: Xu *et al.* (2009). For a related structure, see: Luo *et al.* (2006).



Experimental

Crystal data

$C_7H_5ClN_4$
M_r = 180.60
Monoclinic, $P2/c$
a = 9.4596 (19) Å
b = 11.437 (2) Å
c = 7.2988 (15) Å
β = 107.91 (3)°
V = 751.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 291 K
0.21 × 0.14 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.912, T_{max} = 0.952
7237 measured reflections
1720 independent reflections
1194 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
S = 1.05
1720 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H3···N3	0.85 (1)	2.05 (1)	2.889 (2)	172 (1)
N3—H6···N1	0.83 (3)	2.08 (4)	2.889 (2)	165.7 (2)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2726).

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supplementary materials

Acta Cryst. (2010). E**66**, o742 [**doi:10.1107/S1600536810003788**]

5-(4-Chlorophenyl)-1*H*-tetrazole

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Comment

The tetrazole functional group attracted considerable attention over recent years, because of both the intriguing architectures in coordination chemistry and the potential applications in medicinal chemistry and materials science (Luo *et al.*, 2006). Herein, we reported the synthesis and the crystal structure of the title compound.

In the asymmetric unit of the title compound, $C_7H_5ClN_4$, contains two half molecules of 5-(4-Chlorophenyl)-1*H*-tetrazole. In these two molecules, the centres of bezene and tetrazole rings locate on the symmetry plane, with the dihedral angle of 0.22 (6)° and 17.38 (6)°, respectively.

A one-dimensional chain structure is built up by N—H···N hydrogen bonds between the imino groups of the title compound.

Experimental

For the preparation of the title compound, 4-chlorobenzonitrile (13.7 g, 0.10 mol), ammonium chloride (13.4 g, 0.25 mmol) and NaN3 (7.8 g, 0.12 mol) were dissolved in DMF (120 ml). The mixture was heated to reflux stirred for 24 h under stirring. Then, it was cooled to room temperature and poured into cold water and acidified to pH = 2 with concentrated hydrochloric acid. The suspension was filtrated, and the residue was washed with water and ethanol for several times, and then dried (11.1 g, 61.8 %). Crystals suitable for X-ray analysis were obtained by recrystallization in the EtOH solution.

Refinement

Due to the title compound molecules located on the symmetry planes, the H atoms bound to N atoms were disordered into two positions with the occupancies of 0.5, respectively. H atoms bound to N atoms were located in a difference Fourier map and refined freely. H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic) and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

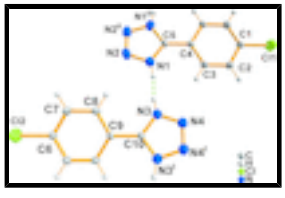

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms. Dashed lines indicate the hydrogen bonds.

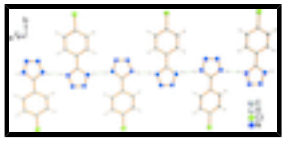

Fig. 2. A partial packing view, showing one-dimensional chain structure. Dashed lines indicate the hydrogen bonds.

5-(4-Chlorophenyl)-1*H*-tetrazole

Crystal data

$C_7H_5ClN_4$	$F(000) = 368$
$M_r = 180.60$	$D_x = 1.596$ Mg m^{-3}
Monoclinic, $P2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yc	Cell parameters from 5352 reflections
$a = 9.4596$ (19) Å	$\theta = 3.1$–$27.5°$
$b = 11.437$ (2) Å	$\mu = 0.45$ mm^{-1}
$c = 7.2988$ (15) Å	$T = 291$ K
$\beta = 107.91$ (3)°	Block, colorless
$V = 751.4$ (3) Å^3	0.21 × 0.14 × 0.11 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	1720 independent reflections
Radiation source: fine-focus sealed tube	1194 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.038$
ω scan	$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{min} = 0.912$, $T_{max} = 0.952$	$k = -14 \rightarrow 14$
7237 measured reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.135$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0807P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1720 reflections	$(\Delta/\sigma)_{max} < 0.001$
118 parameters	$\Delta\rho_{max} = 0.77$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}	Occ. (<1)
C1	0.0000	0.7724 (3)	0.2500	0.0340 (7)	
C2	0.1238 (2)	0.7123 (2)	0.3612 (3)	0.0375 (5)	
H1	0.2067	0.7530	0.4358	0.045*	
C3	0.1235 (2)	0.59197 (19)	0.3606 (3)	0.0331 (5)	
H2	0.2068	0.5518	0.4350	0.040*	
C4	0.0000	0.5293 (3)	0.2500	0.0282 (6)	
C5	0.0000	0.4029 (3)	0.2500	0.0288 (6)	
C6	0.5000	−0.0727 (3)	0.7500	0.0296 (6)	
C7	0.3680 (2)	−0.0135 (2)	0.6704 (3)	0.0389 (5)	
H4	0.2797	−0.0544	0.6188	0.047*	
C8	0.3688 (2)	0.1065 (2)	0.6683 (3)	0.0354 (5)	
H5	0.2809	0.1471	0.6119	0.042*	
C9	0.5000	0.1681 (2)	0.7500	0.0258 (6)	
C10	0.5000	0.2975 (3)	0.7500	0.0267 (6)	
Cl1	0.0000	0.92391 (7)	0.2500	0.0492 (3)	
Cl2	0.5000	−0.22534 (7)	0.7500	0.0464 (3)	
N1	0.1109 (2)	0.33285 (16)	0.3488 (2)	0.0349 (4)	
H3	0.1934	0.3493	0.4318	0.050 (15)*	0.50
N2	0.0660 (2)	0.22079 (17)	0.3089 (3)	0.0418 (5)	
N3	0.3941 (2)	0.36603 (16)	0.6406 (3)	0.0349 (4)	
H6	0.322 (5)	0.352 (4)	0.545 (6)	0.016 (9)*	0.50
N4	0.4364 (2)	0.47685 (17)	0.6842 (3)	0.0398 (5)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0332 (14)	0.0274 (17)	0.0377 (15)	0.000	0.0056 (12)	0.000
C2	0.0313 (10)	0.0320 (12)	0.0424 (11)	−0.0035 (8)	0.0011 (9)	−0.0024 (9)
C3	0.0270 (9)	0.0298 (12)	0.0349 (10)	0.0000 (8)	−0.0016 (8)	0.0017 (8)
C4	0.0267 (13)	0.0285 (17)	0.0270 (13)	0.000	0.0046 (11)	0.000
C5	0.0305 (13)	0.0261 (15)	0.0266 (12)	0.000	0.0038 (11)	0.000
C6	0.0365 (14)	0.0215 (15)	0.0272 (13)	0.000	0.0047 (12)	0.000

C7	0.0324 (11)	0.0310 (12)	0.0456 (12)	−0.0054 (8)	0.0006 (10)	−0.0066 (9)
C8	0.0242 (9)	0.0328 (12)	0.0408 (11)	0.0009 (8)	−0.0021 (8)	−0.0002 (9)
C9	0.0292 (13)	0.0219 (15)	0.0238 (12)	0.000	0.0044 (11)	0.000
C10	0.0248 (12)	0.0282 (16)	0.0244 (12)	0.000	0.0037 (11)	0.000
Cl1	0.0465 (5)	0.0241 (5)	0.0709 (6)	0.000	0.0090 (4)	0.000
Cl2	0.0591 (5)	0.0225 (5)	0.0503 (5)	0.000	0.0061 (4)	0.000
N1	0.0332 (8)	0.0275 (10)	0.0356 (9)	0.0027 (7)	−0.0019 (8)	0.0001 (7)
N2	0.0437 (10)	0.0245 (10)	0.0456 (10)	0.0031 (8)	−0.0036 (8)	0.0027 (8)
N3	0.0329 (9)	0.0257 (10)	0.0374 (9)	0.0008 (7)	−0.0018 (8)	0.0000 (7)
N4	0.0381 (9)	0.0259 (10)	0.0450 (10)	0.0016 (8)	−0.0027 (8)	0.0002 (8)

Geometric parameters (Å, °)

C1—C2	1.385 (3)	C7—C8	1.373 (3)
C1—C2^{i}	1.385 (3)	C7—H4	0.9300
C1—Cl1	1.732 (3)	C8—C9	1.392 (2)
C2—C3	1.376 (3)	C8—H5	0.9300
C2—H1	0.9300	C9—C8^{ii}	1.392 (2)
C3—C4	1.397 (3)	C9—C10	1.480 (4)
C3—H2	0.9300	C10—N3^{ii}	1.328 (3)
C4—C3^{i}	1.397 (3)	C10—N3	1.328 (3)
C4—C5	1.446 (4)	N1—N2	1.353 (3)
C5—N1^{i}	1.340 (3)	N1—H3	0.8492
C5—N1	1.340 (3)	N2—N2^{i}	1.280 (4)
C6—C7^{ii}	1.382 (3)	N3—N4	1.338 (3)
C6—C7	1.382 (3)	N3—H6	0.83 (4)
C6—Cl2	1.746 (3)	N4—N4^{ii}	1.288 (3)
C2—C1—C2^{i}	120.5 (3)	C8—C7—H4	120.4
C2—C1—Cl1	119.77 (15)	C6—C7—H4	120.4
C2^{i}—C1—Cl1	119.77 (15)	C7—C8—C9	120.55 (19)
C3—C2—C1	119.6 (2)	C7—C8—H5	119.7
C3—C2—H1	120.2	C9—C8—H5	119.7
C1—C2—H1	120.2	C8—C9—C8^{ii}	119.2 (3)
C2—C3—C4	121.05 (19)	C8—C9—C10	120.38 (13)
C2—C3—H2	119.5	C8^{ii}—C9—C10	120.38 (14)
C4—C3—H2	119.5	N3^{ii}—C10—N3	107.6 (3)
C3—C4—C3^{i}	118.2 (3)	N3^{ii}—C10—C9	126.18 (13)
C3—C4—C5	120.88 (14)	N3—C10—C9	126.18 (13)
C3^{i}—C4—C5	120.88 (14)	C5—N1—N2	107.97 (18)
N1^{i}—C5—N1	106.6 (3)	C5—N1—H3	130.3
N1^{i}—C5—C4	126.70 (14)	N2—N1—H3	121.5
N1—C5—C4	126.70 (14)	N2^{i}—N2—N1	108.73 (11)
C7^{ii}—C6—C7	121.3 (3)	C10—N3—N4	107.51 (18)
C7^{ii}—C6—Cl2	119.34 (14)	C10—N3—H6	131 (3)
C7—C6—Cl2	119.34 (14)	N4—N3—H6	120 (3)

C8—C7—C6	119.1 (2)	$N4^{ii}$—N4—N3	108.67 (11)

Symmetry codes: (i) −*x*, *y*, −*z*+1/2; (ii) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H3···N3	0.85 (1)	2.05 (1)	2.889 (2)	172.(1)
N3—H6···N1	0.83 (3)	2.08 (4)	2.889 (2)	165.7 (2)

Fig. 1

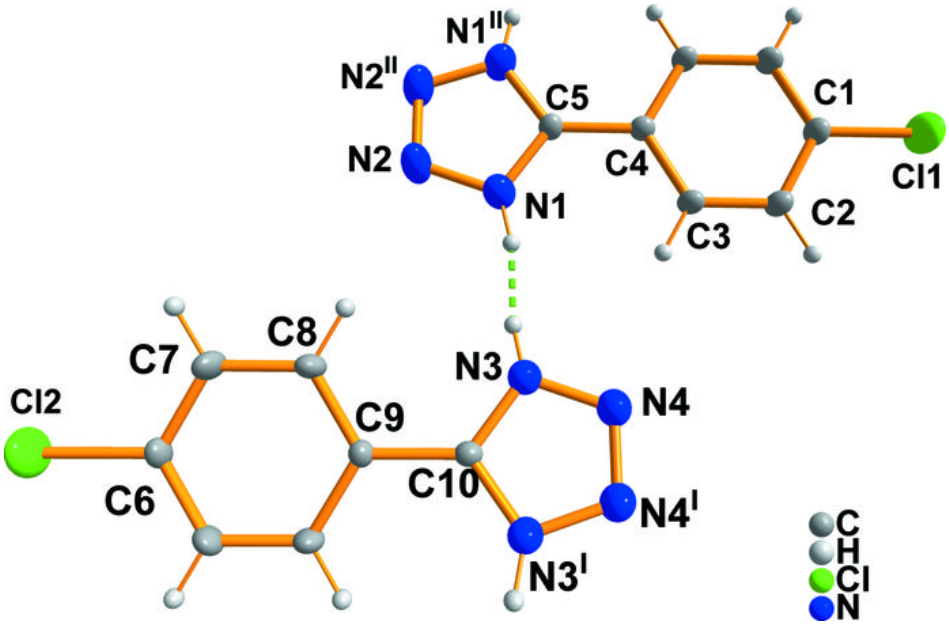
N1II
N2II
C5
C1
N2
C4
Cl1
N1
C2
C3
C8
C7
N3
Cl2
C9
N4
C10
N4I
C6
N3I
C
H
Cl
N

Fig. 2