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5-Chloro-1-phenyl-1*H*-tetrazole

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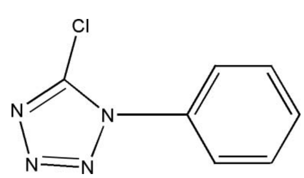
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.092; data-to-parameter ratio = 12.9.

The tetrazole and phenyl rings of the title compound, $C_7H_5ClN_4$, form a dihedral angle 64.5°.

Related literature

For the ferroelectric properties of tetrazole derivatives, see: Sengupta & Mukherjee (2010). For their magnetic properties, see: Grunert *et al.* (2004); Van Koningsbruggen *et al.* (2000). For their luminescent properties, see: Wang *et al.* (2005).



Experimental

Crystal data

$C_7H_5ClN_4$
M_r = 180.60
Monoclinic, $P2_1/n$
a = 7.0428 (7) Å
b = 6.4150 (6) Å
c = 17.5804 (18) Å
β = 96.160 (2)°
V = 789.69 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 296 K
0.15 × 0.14 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998) T_{min} = 0.939, T_{max} = 0.947
3879 measured reflections
1404 independent reflections
1176 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.092
S = 1.05
1404 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2009).

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S1. Comment

The design and synthesis of new tetrazole derivatives have attracted much interest owing to their ferroecletric (Sengupta & Mukherjee, 2010), luminescent (Wang *et al.*, 2005) and magnetic properties (Grunert *et al.*, 2004; Van Koningsbruggen *et al.*, 2000). The crystal structure of 5-chloro-1-phenyl-1*H*-tetrazole (I) is shown in Fig. 1.

S2. Experimental

5-Chloro-1-phenyl-1*H*-tetrazole (I) (54.18 mg, 0.3 mmol) was stirred for 0.5 h in H_2O (5 ml) and CH_3CN (5 ml). Upon slow evaporation of the filtrate at room temperatre for two weeks, well shaped colorless crystals suitable for X-ray diffraction were obtained. Yield: 90%. Elemental analysis calcd (%) for (I): C 46.55, H 2.79, N 31.02%; found: C 46.26, H 2.68, N 31.37%.

S3. Refinement

H atoms were introduced in their idealized positions and refined as riding with C—H 0.93 Å.

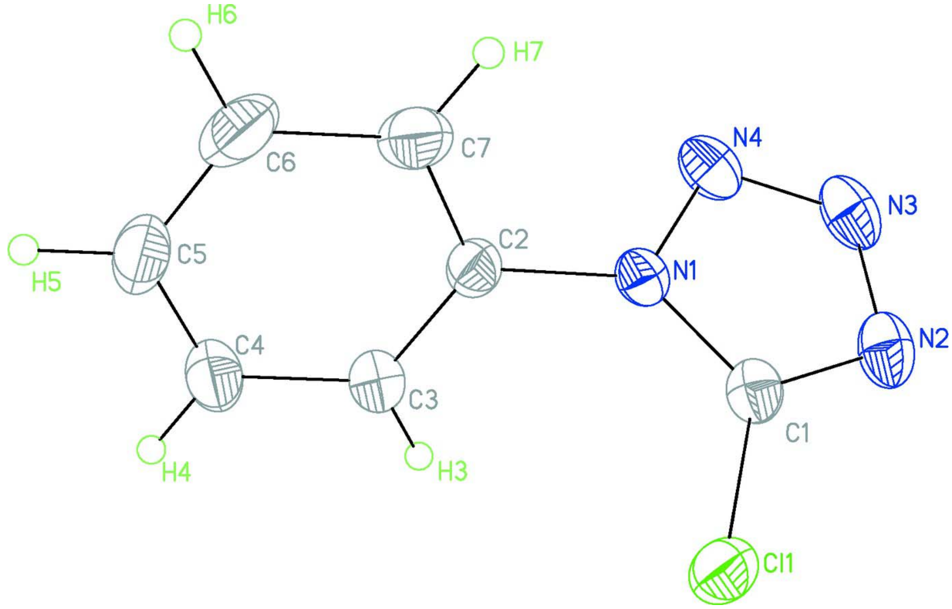

Figure 1

A view of (I), with displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are drawn as circles.

5-Chloro-1-phenyl-1*H*-tetrazole

Crystal data

$C_7H_5ClN_4$
M_r = 180.60
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.0428 (7) Å
b = 6.4150 (6) Å
c = 17.5804 (18) Å
β = 96.160 (2)°
V = 789.69 (13) Å^3
Z = 4
F(000) = 368
D_x = 1.519 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1689 reflections
θ = 3.0–27.2°
μ = 0.43 mm^{-1}
T = 296 K
Block, colourless
0.15 × 0.14 × 0.13 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*; Sheldrick, 1998)
T_{min} = 0.939, T_{max} = 0.947
3879 measured reflections
1404 independent reflections
1176 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −5→8
k = −7→7
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.092
S = 1.05
1404 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.1635P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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}
Cl1	0.15030 (6)	0.26017 (7)	0.03941 (3)	0.05392 (19)
N1	0.5232 (2)	0.25483 (17)	0.08796 (8)	0.0387 (3)
N2	0.4612 (3)	0.24646 (19)	−0.03563 (9)	0.0527 (4)
N3	0.6525 (3)	0.2414 (2)	−0.01533 (10)	0.0558 (4)

N4	0.6930 (2)	0.24610 (19)	0.05813 (10)	0.0504 (4)
C1	0.3852 (3)	0.2547 (2)	0.02910 (10)	0.0416 (4)
C2	0.5109 (2)	0.2662 (2)	0.16905 (9)	0.0417 (4)
C3	0.4356 (2)	0.4431 (3)	0.19789 (9)	0.0505 (4)
H3	0.3949	0.5534	0.1659	0.061*
C4	0.4216 (3)	0.4538 (4)	0.27567 (10)	0.0646 (6)
H4	0.3699	0.5716	0.2963	0.078*
C5	0.4836 (3)	0.2919 (4)	0.32218 (11)	0.0709 (7)
H5	0.4740	0.3003	0.3744	0.085*
C6	0.5600 (3)	0.1167 (4)	0.29252 (11)	0.0725 (6)
H6	0.6029	0.0080	0.3249	0.087*
C7	0.5737 (2)	0.1004 (3)	0.21435 (10)	0.0570 (5)
H7	0.6235	−0.0183	0.1936	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0445 (3)	0.0682 (3)	0.0478 (3)	−0.00030 (19)	−0.0010 (2)	0.00150 (18)
N1	0.0380 (7)	0.0418 (7)	0.0376 (7)	0.0000 (5)	0.0103 (6)	−0.0016 (5)
N2	0.0734 (11)	0.0471 (9)	0.0396 (8)	−0.0045 (7)	0.0160 (8)	−0.0009 (6)
N3	0.0706 (11)	0.0479 (9)	0.0542 (10)	−0.0037 (7)	0.0309 (8)	−0.0039 (6)
N4	0.0477 (8)	0.0495 (8)	0.0577 (10)	−0.0012 (6)	0.0218 (7)	−0.0035 (6)
C1	0.0509 (10)	0.0367 (8)	0.0380 (9)	−0.0018 (6)	0.0083 (8)	0.0009 (6)
C2	0.0345 (8)	0.0559 (10)	0.0350 (8)	−0.0008 (7)	0.0052 (7)	0.0007 (6)
C3	0.0512 (10)	0.0596 (11)	0.0411 (9)	0.0060 (8)	0.0069 (7)	−0.0032 (8)
C4	0.0580 (12)	0.0918 (15)	0.0448 (10)	0.0055 (10)	0.0089 (9)	−0.0151 (10)
C5	0.0493 (11)	0.128 (2)	0.0349 (10)	−0.0011 (12)	0.0031 (8)	0.0015 (11)
C6	0.0518 (12)	0.1107 (18)	0.0532 (11)	0.0097 (12)	−0.0020 (9)	0.0329 (12)
C7	0.0463 (10)	0.0684 (12)	0.0567 (11)	0.0117 (8)	0.0077 (8)	0.0134 (9)

Geometric parameters (Å, º)

Cl1—C1	1.6841 (18)	C3—C4	1.383 (2)
N1—C1	1.341 (2)	C3—H3	0.9300
N1—N4	1.357 (2)	C4—C5	1.364 (3)
N1—C2	1.439 (2)	C4—H4	0.9300
N2—C1	1.309 (2)	C5—C6	1.373 (3)
N2—N3	1.357 (3)	C5—H5	0.9300
N3—N4	1.293 (2)	C6—C7	1.392 (3)
C2—C3	1.373 (2)	C6—H6	0.9300
C2—C7	1.373 (2)	C7—H7	0.9300
C1—N1—N4	107.28 (15)	C4—C3—H3	120.7
C1—N1—C2	130.44 (14)	C5—C4—C3	120.20 (19)
N4—N1—C2	122.27 (14)	C5—C4—H4	119.9
C1—N2—N3	105.02 (16)	C3—C4—H4	119.9
N4—N3—N2	111.63 (15)	C4—C5—C6	120.57 (18)
N3—N4—N1	106.14 (16)	C4—C5—H5	119.7

N2—C1—N1	109.93 (17)	C6—C5—H5	119.7
N2—C1—Cl1	126.31 (16)	C5—C6—C7	120.52 (18)
N1—C1—Cl1	123.75 (14)	C5—C6—H6	119.7
C3—C2—C7	122.63 (16)	C7—C6—H6	119.7
C3—C2—N1	118.32 (14)	C2—C7—C6	117.56 (18)
C7—C2—N1	119.05 (14)	C2—C7—H7	121.2
C2—C3—C4	118.51 (17)	C6—C7—H7	121.2
C2—C3—H3	120.7		

C1—N2—N3—N4	0.03 (16)	N4—N1—C2—C3	115.00 (16)
N2—N3—N4—N1	−0.05 (16)	C1—N1—C2—C7	116.21 (18)
C1—N1—N4—N3	0.04 (15)	N4—N1—C2—C7	−65.26 (19)
C2—N1—N4—N3	−178.79 (12)	C7—C2—C3—C4	−0.4 (3)
N3—N2—C1—N1	−0.01 (15)	N1—C2—C3—C4	179.32 (15)
N3—N2—C1—Cl1	−178.96 (11)	C2—C3—C4—C5	0.7 (3)
N4—N1—C1—N2	−0.02 (16)	C3—C4—C5—C6	−0.1 (3)
C2—N1—C1—N2	178.68 (13)	C4—C5—C6—C7	−0.7 (3)
N4—N1—C1—Cl1	178.96 (10)	C3—C2—C7—C6	−0.4 (3)
C2—N1—C1—Cl1	−2.3 (2)	N1—C2—C7—C6	179.91 (16)
C1—N1—C2—C3	−63.5 (2)	C5—C6—C7—C2	0.9 (3)