Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Xiu Guang Wang and Ying Wang*

Tianjin Key Laboratory of Structure and Performance for Functional Molecules, Tianjin Normal University, Tianjin 300387, People's Republic of China
Correspondence e-mail: hxxywy@mail.tjnu.edu.cn

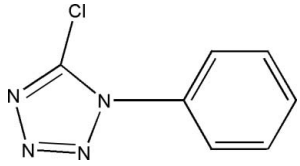
Received 16 April 2011; accepted 2 June 2011

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*.

This work was supported financially by Tianjin Normal University (grant No. 5RL090), the Natural Science Foundation of Tianjin (grant No. 11JCYBJC03600) and the Young Scientist Fund (grant No. 52 G10005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2009).

References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Grunert, C. M., Schweifer, J., Weinberger, P., Linert, W., Mereiter, K., Hilscher, G., Muller, M., Wiesinger, G. & van Koningsbrugger, P. J. (2004). *Inorg. Chem.* **43**, 155–156.
Sengupta, O. & Mukherjee, P. S. (2010). *Inorg. Chem.* **49**, 8583–8590.
Sheldrick, G. M. (1998). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Van Koningsbruggen, P. J., Garcia, Y., Kahn, O., Fournes, L., Kooijman, H., Spek, A. L., Haasnoot, J. G., Moscovici, J., Provost, K., Michalowicz, A., Renz, F. & Gutlich, P. (2000). *Inorg. Chem.* **39**, 1891–1900.
Wang, Z.-X., Lan, Y., Yuan, L.-T. & Liu, C.-Y. (2005). *Acta Cryst.* E**61**, o2033–o2034.

supplementary materials

Acta Cryst. (2011). E**67**, o1633 [**doi:10.1107/S1600536811021210**]

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

X. G. Wang and Y. Wang

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.

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%.

Refinement

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

Figures

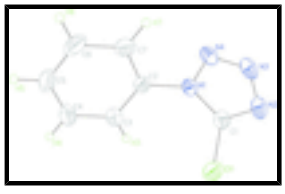


Fig. 1. A view of (I), with displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are drawn as circles.

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

Crystal data

$C_7H_5ClN_4$	$F(000) = 368$
$M_r = 180.60$	$D_x = 1.519$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1689 reflections
$a = 7.0428$ (7) Å	$\theta = 3.0$–$27.2°$
$b = 6.4150$ (6) Å	$\mu = 0.43$ mm^{-1}
$c = 17.5804$ (18) Å	$T = 296$ K
$\beta = 96.160$ (2)°	Block, colourless
$V = 789.69$ (13) Å^3	0.15 × 0.14 × 0.13 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	1404 independent reflections
Radiation source: fine-focus sealed tube	1176 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.014$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)	$h = -5\rightarrow8$
$T_{min} = 0.939$, $T_{max} = 0.947$	$k = -7\rightarrow7$
3879 measured reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.092$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.1635P]$ where $P = (F_o^2 + 2F_c^2)/3$
1404 reflections	$(\Delta/\sigma)_{max} < 0.001$
109 parameters	$\Delta\rho_{max} = 0.12$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ 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 (Å^2)

	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, °)

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)

Fig. 1