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1-Chloro-1*H*-1,2,3-benzotriazole

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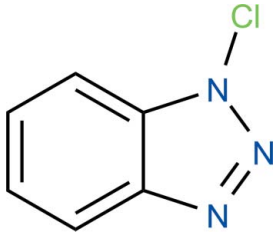
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.068; data-to-parameter ratio = 9.9.

The title compound, $C_6H_4ClN_3$, is essentially planar, with a maximum deviation of 0.007 (3) Å. In the crystal, a short contact of 2.818 (3) Å is observed between N and Cl atoms of adjacent molecules.

Related literature

For related structures of benzotriazole derivatives, see: Jebas *et al.* (2012); Guo *et al.* (2012); Selvarathy *et al.* (2012); Xu & Shen (2012). For applications of the title compound, see: Hunter *et al.* (2006) and references cited therein. For the biological activity of benzotriazole derivatives, see: Gaikwad *et al.* (2012); Dubey *et al.* (2011).



Experimental

Crystal data

$C_6H_4ClN_3$
M_r = 153.57
Orthorhombic, *Fdd*2
a = 22.8022 (11) Å
b = 14.2637 (8) Å
c = 8.2259 (4) Å
V = 2675.4 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 293 K
0.42 × 0.34 × 0.32 mm

Data collection

Agilent Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.979, T_{max} = 1.000
1503 measured reflections
918 independent reflections
867 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.060
S = 1.06
918 reflections
91 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 275 Friedel pairs
Flack parameter: 0.00 (8)

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5634).

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supporting information

Acta Cryst. (2012). E**68**, o3432 [doi:10.1107/S1600536812044820]

1-Chloro-1*H*-1,2,3-benzotriazole

Ming-Yong Yuan, Xia Zhao and Ling-Li Zheng

S1. Comment

Benzotriazole derivates are an important class of heterocylic compounds with essential applications in the organic synthesis and medicinal chemistry. In the synthetic chemistry, 1-chloro-1*H*-benzo[*d*][1,2,3]triazole is an important oxidation and chlorination reagent. Recently, 1-chloro-1*H*-benzo[*d*][1,2,3]triazole has been used in the synthesis of unsymmetrical disulfides (Hunter *et al.*, 2006). Meanwhile, b**e**nzotriazole derivates derivates exhibit numerous essential bioactivitities, especially in antimicrobial (Gaikwad, *et al.*, 2012) and antibubercular activities (Dubey *et al.* 2011). Most recently, several crystal structures of title compound derivates have been reported (Jebas *et al.*, 2012; Guo *et al.*, 2012; Selvarathy *et al.*, 2012; Xu & Shen 2012), but crystal data of 1-chloro-1*H*-benzo[*d*][1,2,3]triazole has not been investigated. Herein, we report the synthesis and crystal structure of the title compound.

The molecular structure of 1-chloro-1*H*-benzo[*d*][1,2,3]triazole is shown in Fig. 1. The bond lengths and angles are within normal ranges. In the crystal, the short contact of 2.818 (3) Å between N and Cl atoms of adjacent molecules occurs.

S2. Experimental

To a stirring solution of benzotriazole (10 g) in 50 ml of 50% acetic acid aqueous solution was added sodium hypochlorite solution (30 ml) at room temperature dropwise. After dropping, the solution was diluted with water (100 ml) to precipitate the product. The mixture was filtered, washed with water to afford 1-chloro-1*H*-benzo[*d*][1,2,3]triazole (8.5 g)as white solid. The single crystals of 1-chloro-1*H*-benzo[*d*][1,2,3]triazole were recrystallized from acetone at room temperature.

S3. Refinement

H atoms were included in idealized positions and refined using a riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

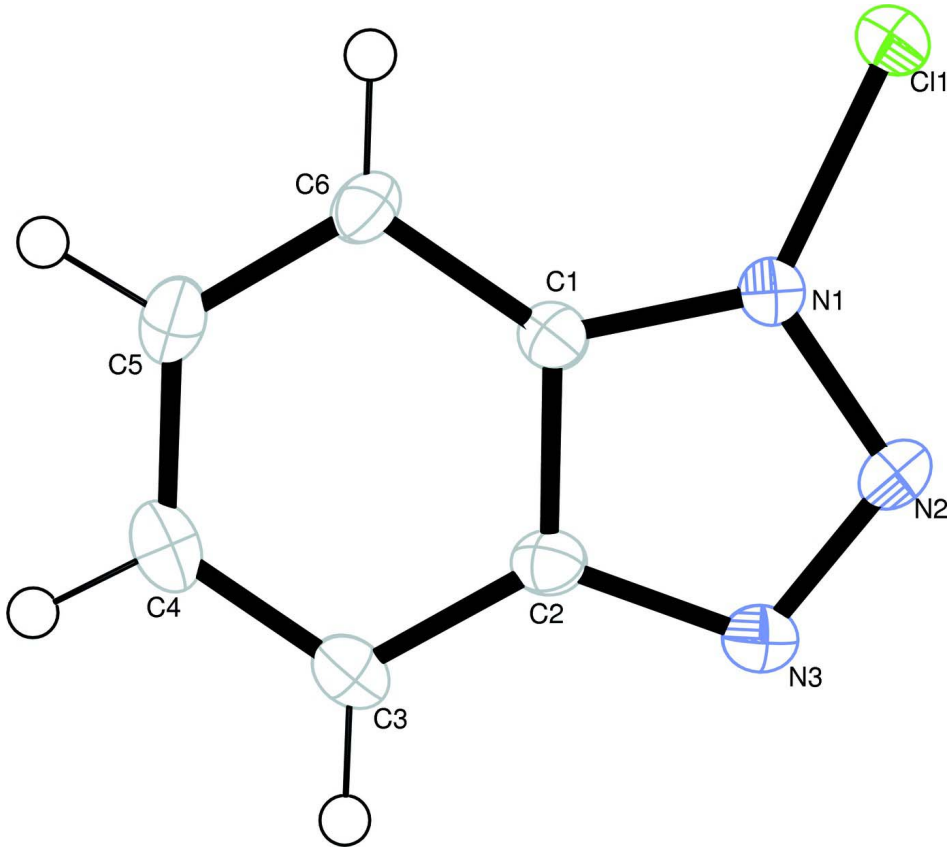

Figure 1

The title compound with displacement ellipsoids drawn at the 50% probability level.

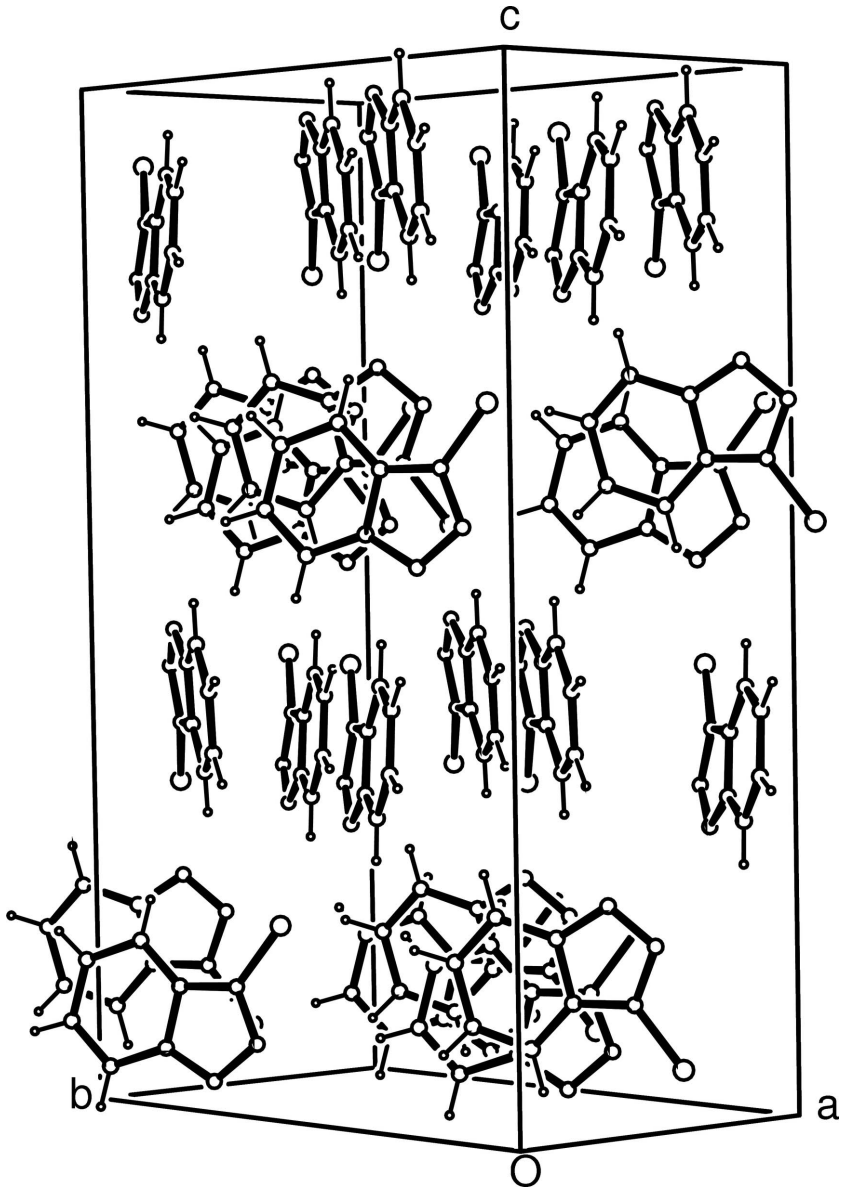

Figure 2

Plane-to-plane stacking of alternate molecules parallel to the *α* axis.

1-Chloro-1*H*-1,2,3-benzotriazole

Crystal data

$C_6H_4ClN_3$
M_r = 153.57
Orthorhombic, *Fdd*2
a = 22.8022 (11) Å
b = 14.2637 (8) Å
c = 8.2259 (4) Å
V = 2675.4 (2) Å^3
Z = 16
F(000) = 1248
D_x = 1.525 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 738 reflections
θ = 3.0–28.5°
μ = 0.48 mm^{-1}
T = 293 K
Block, colourless
0.42 × 0.34 × 0.32 mm

Data collection

Agilent Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0874 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.979, T_{max} = 1.000
1503 measured reflections
918 independent reflections
867 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.2°, θ_{min} = 3.0°
h = −15→27
k = −16→8
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.060
S = 1.06
918 reflections
91 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
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 275 Friedel pairs
Absolute structure parameter: 0.00 (8)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl	0.31785 (3)	0.13250 (5)	−0.13509 (9)	0.0508 (2)
N1	0.37734 (9)	0.18891 (16)	−0.0618 (3)	0.0436 (6)
N2	0.43133 (10)	0.15132 (19)	−0.0788 (3)	0.0544 (7)
N3	0.46849 (10)	0.20933 (18)	−0.0121 (4)	0.0537 (7)
C1	0.37873 (11)	0.27246 (19)	0.0179 (3)	0.0369 (6)
C2	0.43801 (11)	0.2849 (2)	0.0484 (3)	0.0402 (7)
C3	0.45739 (14)	0.3651 (2)	0.1311 (4)	0.0538 (8)
H3	0.4969	0.3751	0.1531	0.065*
C4	0.41526 (15)	0.4282 (2)	0.1780 (4)	0.0577 (9)
H4	0.4265	0.4822	0.2330	0.069*
C5	0.35617 (14)	0.4133 (2)	0.1453 (4)	0.0550 (8)
H5	0.3292	0.4581	0.1796	0.066*
C6	0.33580 (13)	0.3357 (2)	0.0649 (4)	0.0459 (8)
H6	0.2962	0.3262	0.0435	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0413 (4)	0.0522 (4)	0.0587 (4)	−0.0073 (4)	−0.0014 (4)	−0.0109 (4)
N1	0.0307 (12)	0.0452 (15)	0.0549 (15)	−0.0005 (12)	−0.0016 (12)	−0.0116 (13)
N2	0.0396 (15)	0.0519 (17)	0.072 (2)	0.0078 (12)	0.0062 (13)	−0.0114 (15)
N3	0.0327 (12)	0.0566 (16)	0.0719 (16)	0.0032 (14)	−0.0019 (13)	−0.0092 (13)
C1	0.0367 (15)	0.0383 (16)	0.0358 (14)	0.0036 (14)	−0.0016 (12)	0.0000 (13)
C2	0.0368 (15)	0.0404 (16)	0.0434 (14)	−0.0002 (13)	−0.0010 (14)	0.0022 (13)
C3	0.0494 (18)	0.057 (2)	0.0545 (19)	−0.0129 (16)	−0.010 (2)	−0.0014 (17)
C4	0.079 (2)	0.0376 (18)	0.0566 (19)	−0.0060 (18)	−0.002 (2)	−0.0069 (15)
C5	0.0570 (19)	0.0439 (19)	0.064 (2)	0.0099 (16)	0.0071 (18)	−0.0067 (18)
C6	0.0385 (15)	0.0440 (19)	0.0551 (18)	0.0071 (14)	−0.0006 (14)	−0.0004 (16)

Geometric parameters (Å, º)

Cl—N1	1.688 (2)	C3—C4	1.371 (4)
N1—N2	1.350 (3)	C3—H3	0.9300
N1—C1	1.360 (3)	C4—C5	1.390 (4)
N2—N3	1.305 (3)	C4—H4	0.9300
N3—C2	1.376 (4)	C5—C6	1.371 (4)
C1—C2	1.386 (3)	C5—H5	0.9300
C1—C6	1.386 (4)	C6—H6	0.9300
C2—C3	1.403 (4)		
N2—N1—C1	112.1 (2)	C4—C3—H3	121.6
N2—N1—Cl	120.4 (2)	C2—C3—H3	121.6
C1—N1—Cl	127.46 (18)	C3—C4—C5	121.6 (3)
N3—N2—N1	107.3 (2)	C3—C4—H4	119.2
N2—N3—C2	108.7 (2)	C5—C4—H4	119.2
N1—C1—C2	102.8 (2)	C6—C5—C4	123.0 (3)
N1—C1—C6	133.5 (3)	C6—C5—H5	118.5
C2—C1—C6	123.7 (3)	C4—C5—H5	118.5
N3—C2—C1	109.1 (3)	C5—C6—C1	114.9 (3)
N3—C2—C3	131.0 (3)	C5—C6—H6	122.5
C1—C2—C3	120.0 (3)	C1—C6—H6	122.5
C4—C3—C2	116.8 (3)		