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5-Chloro-2-(4-methoxyphenyl)-1,3-benzothiazole

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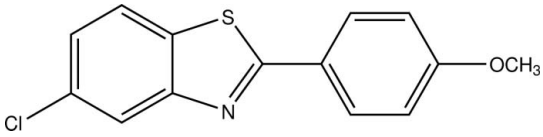
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; R factor = 0.076; wR factor = 0.208; data-to-parameter ratio = 14.0.

In the title compound, $C_{14}H_{10}ClNOS$, the dihedral angle between the benzothiazole ring system and the methoxy-substituted benzene ring is 8.76 (16)°. In the crystal, molecules are stacked in columns along the c axis and no significant intermolecular interactions are observed.

Related literature

For the biological activity of benzothiazole compounds, see: Chohan *et al.* (2003); Khan *et al.* (2011); Hutchinson *et al.* (2002); Burger & Sawhney (1968); Palmer *et al.* (1971). For related structures, see: Yousuf *et al.* (2012*a*,*b*).



Experimental

Crystal data

$C_{14}H_{10}ClNOS$
M_r = 275.74
Orthorhombic, *Pbcn*
a = 29.0274 (16) Å
b = 14.5512 (8) Å
c = 5.8686 (3) Å
V = 2478.8 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 273 K
0.37 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.848, T_{max} = 0.955
13397 measured reflections
2299 independent reflections
1965 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.208
S = 1.15
2299 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*, *PARST* (Nardelli, 1996) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5237).

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supporting information

Acta Cryst. (2013). E**69**, o360 [doi:10.1107/S1600536813001955]

5-Chloro-2-(4-methoxyphenyl)-1,3-benzothiazole

Sammer Yousuf, Shazia Shah, Nida Ambreen, Khalid M. Khan and Shakil Ahmad

S1. Comment

Benzothiazole is a well known class of organic compounds with a diverse range of biological activities (Khan *et al.*, 2011; Chohan *et al.*, 2003, Hutchinson *et al.*, 2002; Burger & Sawhney, 1968; Palmer *et al.*, 1971). The title compound is a methoxy phenyl derivative of benzothiazole synthesized as a part of our ongoing project to synthesize bioactive hetereocyclic compounds.

The crystal structure of title compound (Fig. 1), $C_{16}H_{14}ClNOS$, is similar to that our previously published 5-chloro-2-(3,4,5-trimethoxyphenyl)-1,3-benzothiazole (Yousuf *et al.*, 2012*b*) with the difference that the 3,4,5-trimethoxyphenyl ring is replaced by the 4-methoxyphenyl phenyl ring. The dihedral angle between planner benzothiazole (S1/N1/C1–C7) and methoxy phenyl rings (C8–C13) is 8.76 (16)°. The bond lengths and angle are similar as in previously published benzothiazole compounds (Yousuf *et al.*, 2012*a*,*b*). In the crystal structure the molecules having plane of mirror are arranged in a two-diminesional manner along *a* and *c* axes (Fig. 2).

S2. Experimental

A mixture of 2-amino-4-cholorobenzenethiol (0.159 g, 1 mmol), 4-methoxybenzaldehyde (0.136 g, 1 mmol), sodium metabisulfite (0.2 g) and *N*,*N*-dimethylformamide (10 ml) was refluxed for 2 hrs in a round-bottomed flask. The completion of reaction was monitored by TLC and cool to room temperature followed by addition of cold water to obtain white precipitates. Crystallization from ethanol afforded pure crystal of 5-chloro-2-(4-methoxyphenyl) benzothiazole (yield 0.223 g, 81.1%) found suitable for X-ray diffraction studies.

S3. Refinement

H atoms of phenyl and methyl groups were positioned geometrically with C—H = 0.93 and 0.96 Å, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C_{phenyl}) and 1.5U_{eq}(C_{methyl}). A rotating group model was applied to the methyl group.

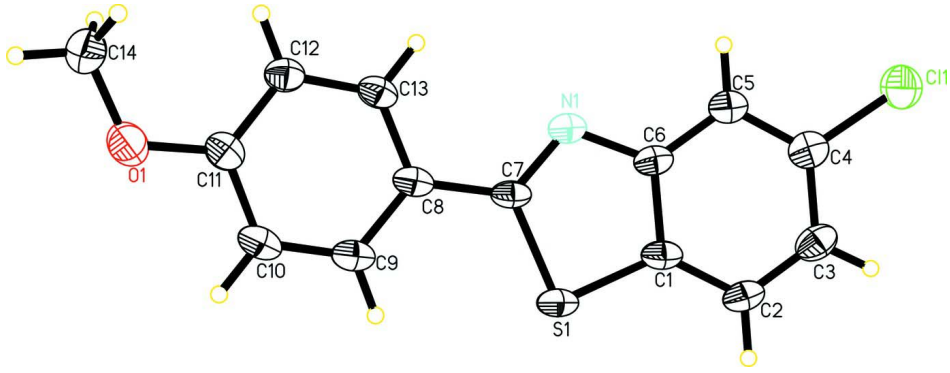

Figure 1

The molecular structure of title compound with displacement ellipsoids drawn at 30% probability level.

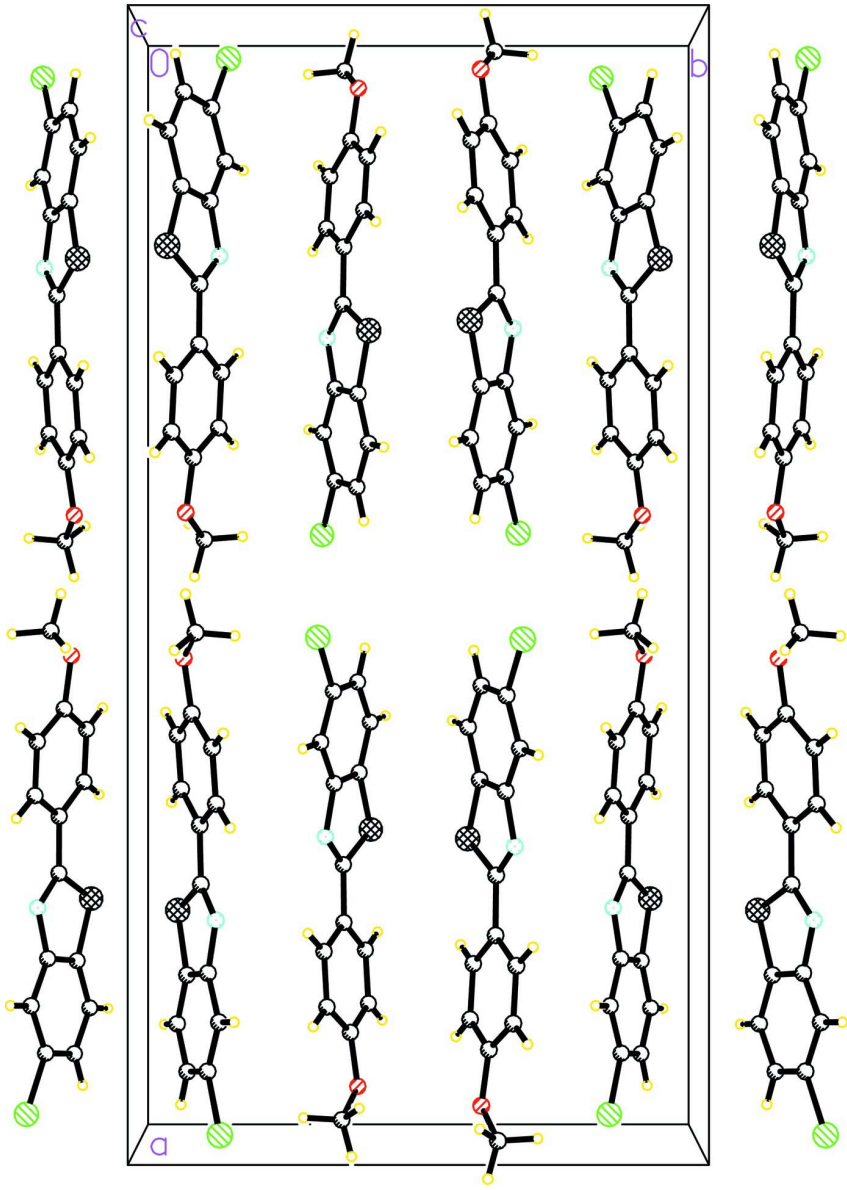

Figure 2

A crystal packing diagram of the title compound, viewed along the *c* axis.

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Crystal data

$C_{14}H_{10}ClNOS$
$M_r = 275.74$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 29.0274\ (16)$ Å
$b = 14.5512\ (8)$ Å
$c = 5.8686\ (3)$ Å
$V = 2478.8\ (2)$ Å^3
$Z = 8$
$F(000) = 1136$
$D_x = 1.478$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3307 reflections
$\theta = 2.5–26.3°$
$\mu = 0.46$ mm^{-1}
$T = 273$ K
Block, colorles
0.37 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.848, T_{max} = 0.955
13397 measured reflections
2299 independent reflections
1965 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.5°, θ_{min} = 1.6°
h = −34→34
k = −17→17
l = −6→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.208
S = 1.15
2299 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0983P)^2 + 3.3682P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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}
Cl1	0.04504 (4)	0.17240 (11)	−0.0360 (2)	0.0787 (5)
S1	0.21904 (4)	0.08514 (7)	0.52664 (16)	0.0494 (4)
O1	0.43838 (11)	0.1057 (2)	0.1916 (6)	0.0656 (9)
N1	0.21907 (12)	0.1613 (2)	0.1301 (5)	0.0437 (8)
C1	0.16642 (15)	0.1048 (2)	0.4009 (6)	0.0450 (9)
C2	0.12234 (17)	0.0857 (3)	0.4807 (7)	0.0502 (10)
H2A	0.1179	0.0592	0.6231	0.060*
C3	0.08560 (16)	0.1072 (3)	0.3433 (7)	0.0556 (11)
H3A	0.0558	0.0946	0.3927	0.067*
C4	0.09246 (15)	0.1475 (3)	0.1304 (8)	0.0530 (10)
C5	0.13595 (15)	0.1688 (3)	0.0488 (7)	0.0471 (9)
H5A	0.1400	0.1968	−0.0922	0.057*
C6	0.17346 (14)	0.1466 (2)	0.1872 (6)	0.0420 (9)
C7	0.24620 (14)	0.1318 (2)	0.2888 (6)	0.0409 (9)
C8	0.29667 (14)	0.1305 (2)	0.2692 (6)	0.0420 (9)
C9	0.32493 (16)	0.0941 (3)	0.4380 (7)	0.0511 (10)

H9A	0.3118	0.0730	0.5727	0.061*
C10	0.37175 (16)	0.0885 (3)	0.4104 (7)	0.0535 (11)
H10A	0.3901	0.0646	0.5261	0.064*
C11	0.39169 (15)	0.1187 (3)	0.2077 (7)	0.0487 (10)
C12	0.36468 (15)	0.1576 (3)	0.0376 (7)	0.0479 (9)
H12A	0.3780	0.1795	−0.0959	0.057*
C13	0.31762 (15)	0.1631 (2)	0.0709 (7)	0.0461 (9)
H13A	0.2994	0.1893	−0.0421	0.055*
C14	0.46063 (17)	0.1316 (4)	−0.0114 (9)	0.0717 (14)
H14A	0.4926	0.1149	−0.0032	0.108*
H14B	0.4580	0.1969	−0.0316	0.108*
H14C	0.4465	0.1007	−0.1379	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0538 (7)	0.1036 (11)	0.0787 (9)	0.0116 (7)	0.0019 (6)	0.0106 (7)
S1	0.0692 (7)	0.0454 (6)	0.0336 (5)	−0.0036 (5)	0.0005 (4)	0.0084 (4)
O1	0.0598 (19)	0.072 (2)	0.065 (2)	0.0054 (15)	−0.0097 (16)	0.0031 (16)
N1	0.058 (2)	0.0384 (16)	0.0347 (16)	−0.0028 (14)	0.0022 (15)	0.0019 (13)
C1	0.069 (3)	0.0347 (18)	0.0308 (18)	−0.0014 (17)	0.0019 (18)	0.0005 (14)
C2	0.068 (3)	0.044 (2)	0.039 (2)	−0.0038 (19)	0.0129 (19)	0.0029 (16)
C3	0.066 (3)	0.051 (2)	0.050 (2)	−0.004 (2)	0.020 (2)	−0.0059 (19)
C4	0.061 (3)	0.046 (2)	0.052 (2)	0.0044 (18)	0.007 (2)	−0.0042 (18)
C5	0.061 (2)	0.0386 (19)	0.042 (2)	0.0006 (17)	0.0043 (19)	−0.0007 (16)
C6	0.061 (2)	0.0313 (16)	0.0334 (18)	−0.0018 (16)	0.0071 (17)	−0.0023 (14)
C7	0.064 (2)	0.0315 (17)	0.0269 (17)	−0.0024 (16)	0.0010 (17)	−0.0002 (14)
C8	0.065 (2)	0.0298 (16)	0.0314 (18)	−0.0007 (15)	−0.0052 (17)	−0.0006 (14)
C9	0.072 (3)	0.045 (2)	0.036 (2)	−0.0032 (19)	−0.0038 (19)	0.0056 (16)
C10	0.071 (3)	0.047 (2)	0.043 (2)	0.0017 (19)	−0.016 (2)	0.0052 (17)
C11	0.056 (2)	0.043 (2)	0.047 (2)	0.0021 (17)	−0.0078 (19)	−0.0040 (17)
C12	0.059 (2)	0.042 (2)	0.043 (2)	−0.0012 (18)	−0.0009 (18)	0.0047 (16)
C13	0.061 (2)	0.0376 (19)	0.040 (2)	0.0003 (17)	−0.0088 (18)	0.0040 (15)
C14	0.055 (3)	0.092 (4)	0.068 (3)	−0.007 (3)	0.001 (2)	0.004 (3)

Geometric parameters (Å, º)

Cl1—C4	1.726 (5)	C5—H5A	0.9300
S1—C1	1.720 (4)	C7—C8	1.470 (6)
S1—C7	1.741 (4)	C8—C9	1.391 (5)
O1—C11	1.372 (5)	C8—C13	1.396 (5)
O1—C14	1.407 (5)	C9—C10	1.371 (7)
N1—C7	1.293 (5)	C9—H9A	0.9300
N1—C6	1.382 (5)	C10—C11	1.394 (6)
C1—C2	1.391 (6)	C10—H10A	0.9300
C1—C6	1.409 (5)	C11—C12	1.390 (5)
C2—C3	1.373 (7)	C12—C13	1.382 (6)
C2—H2A	0.9300	C12—H12A	0.9300

C3—C4	1.394 (6)	C13—H13A	0.9300
C3—H3A	0.9300	C14—H14A	0.9600
C4—C5	1.386 (6)	C14—H14B	0.9600
C5—C6	1.396 (6)	C14—H14C	0.9600
C1—S1—C7	89.62 (18)	C9—C8—C13	117.8 (4)
C11—O1—C14	118.4 (4)	C9—C8—C7	122.5 (4)
C7—N1—C6	110.9 (3)	C13—C8—C7	119.7 (3)
C2—C1—C6	121.3 (4)	C10—C9—C8	121.5 (4)
C2—C1—S1	129.8 (3)	C10—C9—H9A	119.2
C6—C1—S1	109.0 (3)	C8—C9—H9A	119.2
C3—C2—C1	118.2 (4)	C9—C10—C11	119.6 (4)
C3—C2—H2A	120.9	C9—C10—H10A	120.2
C1—C2—H2A	120.9	C11—C10—H10A	120.2
C2—C3—C4	120.7 (4)	O1—C11—C12	124.4 (4)
C2—C3—H3A	119.6	O1—C11—C10	115.2 (4)
C4—C3—H3A	119.6	C12—C11—C10	120.5 (4)
C5—C4—C3	122.3 (4)	C13—C12—C11	118.7 (4)
C5—C4—Cl1	118.9 (3)	C13—C12—H12A	120.7
C3—C4—Cl1	118.8 (3)	C11—C12—H12A	120.7
C4—C5—C6	117.2 (4)	C12—C13—C8	121.9 (4)
C4—C5—H5A	121.4	C12—C13—H13A	119.0
C6—C5—H5A	121.4	C8—C13—H13A	119.0
N1—C6—C5	124.7 (3)	O1—C14—H14A	109.5
N1—C6—C1	114.9 (4)	O1—C14—H14B	109.5
C5—C6—C1	120.3 (4)	H14A—C14—H14B	109.5
N1—C7—C8	123.7 (3)	O1—C14—H14C	109.5
N1—C7—S1	115.5 (3)	H14A—C14—H14C	109.5
C8—C7—S1	120.6 (3)	H14B—C14—H14C	109.5
C7—S1—C1—C2	179.4 (4)	C1—S1—C7—N1	1.1 (3)
C7—S1—C1—C6	−0.7 (3)	C1—S1—C7—C8	−174.8 (3)
C6—C1—C2—C3	1.2 (6)	N1—C7—C8—C9	−176.7 (3)
S1—C1—C2—C3	−178.9 (3)	S1—C7—C8—C9	−1.1 (5)
C1—C2—C3—C4	−0.4 (6)	N1—C7—C8—C13	0.5 (5)
C2—C3—C4—C5	−0.9 (6)	S1—C7—C8—C13	176.0 (3)
C2—C3—C4—Cl1	179.6 (3)	C13—C8—C9—C10	−1.2 (6)
C3—C4—C5—C6	1.3 (6)	C7—C8—C9—C10	176.0 (4)
Cl1—C4—C5—C6	−179.2 (3)	C8—C9—C10—C11	−0.9 (6)
C7—N1—C6—C5	−178.4 (3)	C14—O1—C11—C12	−1.3 (6)
C7—N1—C6—C1	0.7 (4)	C14—O1—C11—C10	177.8 (4)
C4—C5—C6—N1	178.6 (3)	C9—C10—C11—O1	−176.6 (4)
C4—C5—C6—C1	−0.4 (5)	C9—C10—C11—C12	2.5 (6)
C2—C1—C6—N1	−179.9 (3)	O1—C11—C12—C13	177.1 (4)
S1—C1—C6—N1	0.2 (4)	C10—C11—C12—C13	−1.9 (6)
C2—C1—C6—C5	−0.8 (5)	C11—C12—C13—C8	−0.2 (6)
S1—C1—C6—C5	179.3 (3)	C9—C8—C13—C12	1.8 (5)
C6—N1—C7—C8	174.5 (3)	C7—C8—C13—C12	−175.5 (3)

C6—N1—C7—S1	−1.2 (4)