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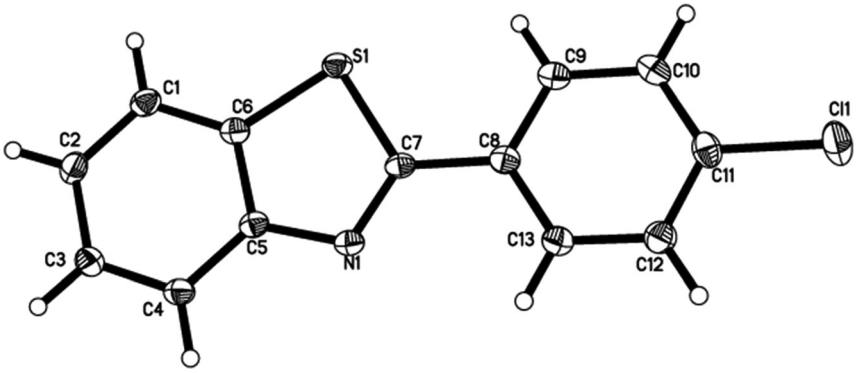
Crystal structure of 2-(4-chlorophenyl) benzothiazole, $C_{13}H_8ClNS$



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Abstract

$C_{13}H_8ClNS$, monoclinic, $P21/c$ (no. 14), a = 11.0497(5) Å, b = 14.1040(6) Å, c = 7.1466(3) Å, β = 98.556(4)°, V = 1101.37(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0298, $wR_{ref}(F^2)$ = 0.0815, T = 150 K.

CCDC no.: 2419729

The crystal structure is shown in the figure. Table 1 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.14 × 0.10 × 0.07 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.50 mm^{-1}
Diffractometer, scan mode:	Oxford Excalibur, ω scan
θ_{max}, completeness:	26.4°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9483, 2246, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1944
$N(param)_{refined}$:	145
Programs:	Oxford,[1] Olex2,[2] SHELX[3]

1 Source of material

A mixture of o-aminothiophenol (0.0624 g, 0.5 mmol), 4-chlorobenzaldehyde (0.0703 g, 0.5 mmol), and tetrabutylammonium tetrafluoroborate (20 mol%) was dissolved in ethanol (5 mL). A carbon rod was used as the anode, and a platinum sheet served as the cathode in the electrolytic cell. The reaction mixture was stirred at room temperature while a constant current of 10 mA was applied for 20 min. After completion, the mixture was washed with saturated brine and extracted with EtOAc. The organic layers were dried over anhydrous Na_2SO_4, concentrated under reduced pressure, and the residue was purified by flash column chromatography to afford the desired product. Melting point: 118 °C.

2 Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Discussion

2–Aryl-benzothiazoles are an important class of nitrogen-containing heterocyclic compounds that have been widely applied in the agricultural field due to their insecticidal and antifungal bioactivities.[4,5] In the pharmaceutical field, they exhibit antitumor and antitubercular effects.[6,7] Additionally,

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2-(4-chlorophenyl)benzothiazole and its derivatives are also structural units for synthesizing optical materials, which can be used in luminescent devices[8] and fluorescent probes.[9] The molecular structure of a compound determines its properties. Therefore, the investigation on the crystal structures of benzothiazoles has received wide attention.[10,11] However, the crystal structure of halogenated benzothiazole derivatives is less studied.[12]

The asymmetric unit contains one molecule of the title compound, which is constructed by a benzothiazole and 4-chlorophenyl molecules (see the Figure). The benzothiazole together with the 4-chlorophenyl molecule is almost in a strict plane, the dihedral angle between the benzothiazole and the 4-chlorophenyl molecule is found to be 4.4°. The N(1)–C(5)–C(6)–S(1) and C(5)–N(1)–C(7)–S(1) torsion angles are 0.50(16)° and 0.33(16)°. The N(1)–C(7)–C(8)–C(13) and S(1)–C(7)–C(8)–C(13) torsion angles are −2.80(2)° and 175.27(11)°. The C(6)–S(1)–C(7) and C(7)–N(1)–C(5) bond angle are 89.17(7)° and 110.73(13)°. The N(1)–C(7)–C(8) and C(10)–C(11)–Cl(1) bond angles are 124.26(14)° and 119.04(13)°. The distances in sulfur-carbon bonds and nitrogen-carbon bonds are 1.7285(16) Å for S(1)–C(6), 1.7558(15) Å for S(1)–C(7), 1.3875(19) Å for N(1)–C(5), and 1.3009(19) Å for N(1)–C(7), respectively. The 4-chlorophenyl group is connected to the benzothiazole ring through a C–C bond, leading to the more stable structure, which is similar to the stereo-configuration of the compound reported in the references.[12] The bond lengths and angles are all in the expected ranges. Interestingly for the title compound another polymorph, crystalline solid has been already reported.[13]

The complete set of X-ray diffraction data for the title compound was deposited to the Cambridge Crystallographic Data Centre (CCDC entry No.2419729).

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