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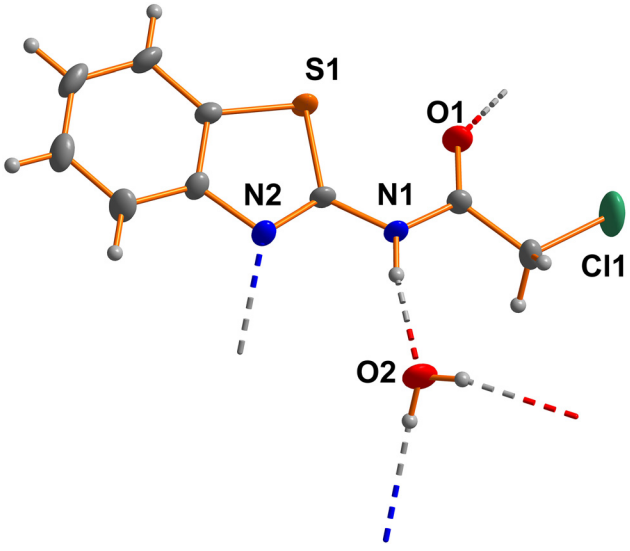
Crystal structure of *N*-(benzo[*d*]thiazol-2-yl)-2-chloroacetamide, $C_9H_7ClN_2OS$



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Abstract

$C_9H_7ClN_2OS$, monoclinic, $P2_1/n$ (no. 14), a = 8.3507(3) Å, b = 12.3768(4) Å, c = 10.2340(4) Å, β = 96.857(4)°, V = 1050.17(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0673, $wR_{ref}(F^2)$ = 0.2013, T = 296(2) K.

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The crystal structure is shown in the figure above. Tables 1–2 contain details of the measurement method and a list of atoms including atomic coordinates and displacement parameters.

1 Source of material

1.0 g(6.66 mmol) 2-aminobenzothiazole, 1.06 ml (13.32 mmol) chloroacetyl chloride and 20 ml tetrahydrofuran were added to a 250 ml round flask and stirred to dissolve, stirred at room temperature for 2 h. After the reaction was completed, poured the reaction liquid into a 500 ml beaker, added an appropriate amount of distilled water, precipitate the solid, and then filter the solid after precipitation. By recrystallization of anhydrous ethanol gave the white solid (1.31 g, 86.8 %). ^{1}H NMR (600 MHz, $CDCl_3$) d 7.82 (s, 1H), 7.48 (s, 1H), 7.84 (s, 1H), 7.36 (s, 1H), 4.32 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) d 164.43, 156.60, 152.07, 126.53, 126.27, 124.52, 121.52, 121.43, 42.11. MS (ESI): m/z = 227.0030 $[M+H]^+$. FTIR (KBr, cm^{-1}) 3506.54 (nNH secondary amine), 3381.16 (nNH acylamino), 2920.18 (nCH methylene), 2864.25 (nasCH methylene), 1693.48 (nC=O carbonyl), 1597.04 (nC=N thiazole), 1562.32 (nasC-C benzene), 1176.56 (nCH benzene), 773.44 (nCCl).

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ:	4.94 mm^{-1}
Diffractometer, scan mode:	New Gemini, ω
θ_{max}, completeness:	72.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3775, 2021, 0.063
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1734
$N(param)_{refined}$:	144
Programs:	SHELX[1,3], Olex2[2]

2 Experimental details

The carbon-bound hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

Benzothaizole (BTA) is a fused benzoheterocyle which is present in many naturally occurring products and is responsible for the medicinal, pharmacological and pharmaceutical applications of such natural products.[4] Benzothiazole is a heterocyclic organic compound with a wide range of biological activities.[5–9]

The basic structure of the title compound is a benzothiazole. The key lengths and angles obtained from the title

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.31615 (14)	0.93636 (7)	0.54550 (10)	0.0520 (4)
S1	0.55038 (9)	0.53525 (6)	0.73413 (7)	0.0265 (3)
O1	0.4705 (3)	0.74346 (19)	0.6681 (2)	0.0338 (6)
N1	0.3053 (3)	0.6184 (2)	0.5616 (2)	0.0222 (6)
N2	0.3123 (3)	0.4335 (2)	0.5997 (2)	0.0227 (6)
C00A	0.2488 (4)	0.8039 (2)	0.5109 (3)	0.0281 (7)
H00A	0.138843	0.796718	0.531461	0.034*
H00B	0.248728	0.789664	0.417658	0.034*
C1	0.3752 (4)	0.5285 (2)	0.6236 (3)	0.0200 (6)
C2	0.4064 (4)	0.3556 (2)	0.6712 (3)	0.0221 (6)
C3	0.3761 (4)	0.2443 (3)	0.6676 (3)	0.0289 (7)
H3	0.287502	0.216333	0.614633	0.035*
C4	0.4802 (4)	0.1769 (3)	0.7442 (3)	0.0326 (8)
H4	0.459930	0.103026	0.743973	0.039*
C5	0.6156 (4)	0.2176 (3)	0.8221 (3)	0.0332 (8)
H5	0.684539	0.170482	0.872398	0.040*
C6	0.6483 (4)	0.3276 (3)	0.8252 (3)	0.0305 (7)
H6	0.738299	0.354831	0.877074	0.037*
C007	0.3539 (4)	0.7216 (2)	0.5888 (3)	0.0217 (6)
C7	0.5426 (3)	0.3963 (3)	0.7485 (3)	0.0226 (6)
O2	0.0328 (3)	0.5976 (2)	0.3794 (3)	0.0422 (7)
H2A	−0.063869	0.592092	0.396973	0.063*
H2B	0.034887	0.636194	0.310951	0.063*
H1	0.223 (5)	0.604 (3)	0.514 (4)	0.021 (9)*

structure are within the normal range and are consistent with those previously reported in similar structures.[10,11] The compound is prepared by the reaction of 2-aminobenzothiazole with chloroacetyl chloride. The crystal structure proves that the compound has been successfully acylated, and the bond length of the C=O bond is 1.221(6) Å. The benzothiazole ring and the phenyl ring have a dihedral angle of 0.18°. The nitrogen atom of the amide bond and the oxygen atom of the water form the intermolecular hydrogen bonds (see the figure).

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