Eric C. Hosten and Richard Betz*

The crystal structure of 2-methyl- β -naphthothiazole, $C_{12}H_9NS$

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Abstract

$C_{12}H_9NS$, monoclinic, $P2_1/n$ (no. 14), $a = 5.0743(5)$ Å, $b = 14.0545(13)$ Å, $c = 13.3319(17)$ Å, $\beta = 91.102(5)^\circ$, $V = 950.61(18)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0322$, $wR_{ref}(F^2) = 0.0908$, $T = 200$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was obtained commercially (Aldrich). Crystals suitable for the diffraction study were taken directly from the provided product.

*Corresponding author: Richard Betz, Department of Chemistry, Nelson Mandela University, Summerstrand Campus (South), University Way, Summerstrand, PO Box 77000, Port Elizabeth 6031, South Africa, E-mail: Richard.Betz@mandela.ac.za. <https://orcid.org/0000-0002-5730-2152>

Eric C. Hosten, Department of Chemistry, Nelson Mandela University, Summerstrand Campus (South), University Way, Summerstrand, PO Box 77000, Port Elizabeth 6031, South Africa. <https://orcid.org/0000-0003-4173-2550>

Table 1: Data collection and handling.

Crystal:	Colourless rod
Size:	$0.51 \times 0.16 \times 0.15$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.29 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.3° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8686, 2362, 0.016
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1970
$N(\text{param})_{\text{refined}}$:	128
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.07674 (7)	0.54027 (2)	0.34013 (3)	0.03267 (12)
N1	0.3017 (2)	0.65777 (8)	0.21966 (8)	0.0284 (2)
C1	0.3210 (3)	0.61354 (9)	0.38975 (10)	0.0277 (3)
C2	0.4172 (2)	0.67089 (9)	0.31371 (9)	0.0253 (3)
C3	0.6188 (2)	0.73913 (9)	0.33517 (9)	0.0257 (3)
C4	0.7265 (3)	0.79895 (9)	0.26118 (10)	0.0319 (3)
H4	0.662560	0.795418	0.193841	0.038*
C5	0.9229 (3)	0.86201 (10)	0.28632 (12)	0.0378 (3)
H5	0.995423	0.901586	0.236096	0.045*
C6	1.0178 (3)	0.86860 (10)	0.38565 (12)	0.0386 (3)
H6	1.153997	0.912616	0.402151	0.046*
C7	0.9158 (3)	0.81215 (10)	0.45886 (11)	0.0350 (3)
H7	0.980988	0.817627	0.525882	0.042*
C8	0.7141 (3)	0.74565 (9)	0.43589 (10)	0.0285 (3)
C9	0.6072 (3)	0.68570 (10)	0.51133 (10)	0.0346 (3)
H9	0.671240	0.691425	0.578481	0.041*
C10	0.4157 (3)	0.62047 (10)	0.48966 (11)	0.0344 (3)
H10	0.347748	0.580634	0.540592	0.041*
C11	0.1199 (3)	0.59290 (9)	0.22273 (10)	0.0295 (3)
C12	−0.0522 (3)	0.56580 (12)	0.13503 (12)	0.0393 (3)
H12A	0.021903	0.591642	0.073401	0.059*
H12B	−0.229527	0.591685	0.144048	0.059*
H12C	−0.061872	0.496305	0.130160	0.059*

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å for aromatic carbon atoms) and were included

in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

The H atoms of the methyl group were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density (HFIX 137 in the *SHELX* program suite [3]), with $U(\text{H})$ set to $1.5U_{\text{eq}}(\text{C})$.

Comment

Heterocyclic compounds have attracted attention in modern pharmaceutical research due to their varied beneficial effects in fighting diseases. But while the traditional way of developing new medications rests on trial-and-error with regards to finding promising classes of molecules a more rational design of modern drugs tries to leverage structure-effect relationships. The latter requires sound structural information about the metrical parameters of such compounds. In continuation of our own interest in the structural variety of benzo-annealed heterocyclic compounds [7–22], the molecular and crystal structure of the title compound were determined. The structures of several benzothiazole derivatives have been published previously [23–25].

The title structure shows a derivative of naphthalene featuring a thiazole ring annealed in β position [26]. A methyl group is bonded to the carbon atom located between the pnictogen and the chalcogen atom. The C–N bond lengths of 1.2984(17) and 1.3861(17) Å and the C–S bond lengths of 1.7328(14) and 1.7487(14) Å are found in the typical range apparent for other benzothiazole derivatives whose metrical parameters have been deposited with the Cambridge Structural Database [27]. The molecule is essentially planar with the least-squares plane as defined by all non-hydrogen atoms showing a maximum deviation of only 0.073(2) Å for the exocyclic carbon atom from this common plane.

The crystal structure of the title compound is marked by an absence of intermolecular contacts whose range falls by at least 0.1 Å below the sum of van-der-Waals radii of the atoms participating in them. The major stabilizing contribution stems from π stacking between the heterocyclic moiety as well as the ring of the naphthalene scaffold that does not bear the annealed heterocycle in a symmetry-generated neighbouring molecule. The distance between these latter two centers of gravity was measured at 3.5470(9) Å.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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