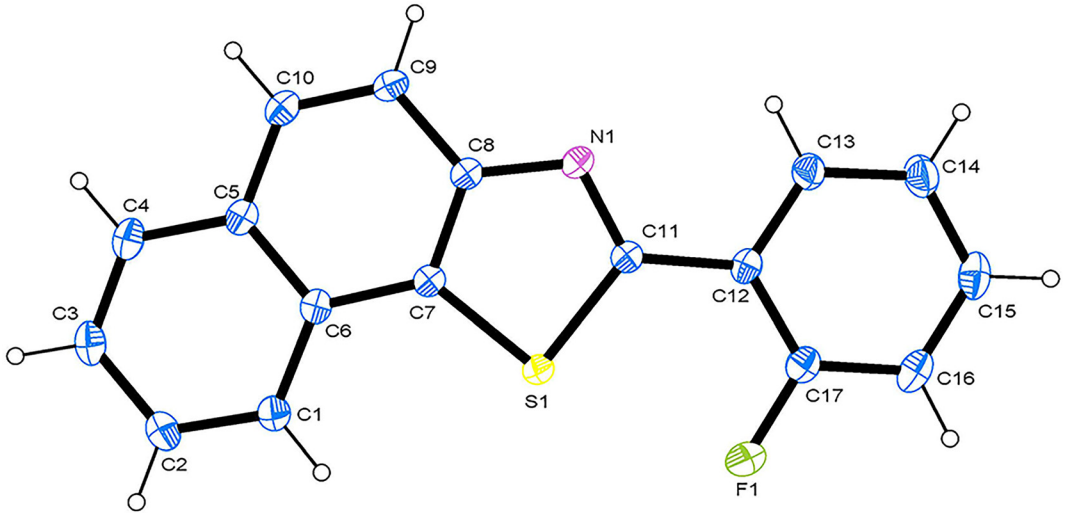
Xiaoming Zhu* and Hongsheng Jin

The crystal structure of 2-(2-fluorophenyl)naphtho[2,1-*d*]thiazole, $C_{17}H_{10}FNS$



https://doi.org/10.1515/ncrs-2023-0183
Received April 14, 2023; accepted May 8, 2023;
published online May 18, 2023

Abstract

$C_{17}H_{10}FNS$, monoclinic, $P2_1/n$ (no. 14), a = 6.1859(2) Å, b = 10.7071(2) Å, c = 19.4475(4) Å, β = 95.794(2)°, V = 1281.49(5) Å^3, Z = 4, $R_{gt}(F)$ = 0.0476, $wR_{ref}(F^2)$ = 0.1333, T = 296 (2) K.

CCDC no.: 2244942

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.

1 Source of material

The title compound was prepared according to our previous synthesis method [5]. Crystals were obtained by slow evaporation from a dichloromethane solution at room temperature.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.27 × 0.25 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	2.24 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	67.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7053, 2311, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 2100
$N(param)_{refined}$:	181
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], WinGX/ORTEP [4]

2 Experimental details

All H-atoms bonded to C atoms were placed geometrically and refined using a riding model with common isotropic displacement factors U_{iso}(H) = 1.2 or 1.5 U_{eq} (parent C-atom).

3 Comment

Benzothiazoles constitute the key moiety of many natural products and pharmaceutical drugs, and show their good biological activities [6, 7]. The naphthalene derivatives are present in bioactive compounds, featuring a wide range of activities such as antihypertensive, anti-inflammatory,

***Corresponding author: Xiaoming Zhu**, School of Chemistry and Materials Science, Hengyang Normal University, Hengyang, Hunan 421008, China, E-mail: zxmhnhy@hynu.edu.cn. https://orcid.org/0000-0003-4086-4674
Hongsheng Jin, Yueyun Middle School, Hengyang, Hunan 421900, China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1	1.11946 (8)	0.64595 (5)	0.40042 (3)	0.0378 (2)
C17	1.1939 (4)	0.8572 (2)	0.51990 (13)	0.0456 (5)
F1	1.3354 (2)	0.83864 (15)	0.47229 (9)	0.0685 (5)
N1	0.7883 (3)	0.61116 (16)	0.46839 (9)	0.0364 (4)
C1	1.1088 (4)	0.4487 (2)	0.27074 (12)	0.0447 (5)
H1	1.220011	0.507306	0.276838	0.054*
C2	1.1054 (4)	0.3643 (2)	0.21744 (14)	0.0535 (6)
H2	1.214658	0.365976	0.187912	0.064*
C3	0.9390 (4)	0.2762 (2)	0.20732 (13)	0.0540 (6)
H3	0.937730	0.219457	0.171071	0.065*
C4	0.7789 (4)	0.2730 (2)	0.25024 (13)	0.0490 (6)
H4	0.669176	0.213646	0.243000	0.059*
C5	0.7757 (3)	0.35788 (18)	0.30549 (11)	0.0385 (5)
C6	0.9458 (3)	0.44726 (18)	0.31620 (10)	0.0357 (5)
C7	0.9388 (3)	0.52981 (18)	0.37335 (10)	0.0337 (4)
C8	0.7741 (3)	0.52493 (18)	0.41651 (10)	0.0344 (5)
C9	0.6052 (3)	0.4346 (2)	0.40453 (12)	0.0427 (5)
H9	0.493770	0.430555	0.433196	0.051*
C10	0.6098 (4)	0.3551 (2)	0.35077 (13)	0.0451 (6)
H10	0.499681	0.296081	0.343134	0.054*
C11	0.9596 (3)	0.68195 (19)	0.46716 (10)	0.0342 (5)
C12	1.0102 (3)	0.78225 (18)	0.51771 (11)	0.0371 (5)
C13	0.8690 (4)	0.8046 (2)	0.56739 (12)	0.0475 (6)
H13	0.743421	0.756820	0.567487	0.057*
C14	0.9116 (5)	0.8965 (2)	0.61672 (15)	0.0594 (7)
H14	0.814932	0.910341	0.649561	0.071*
C15	1.0977 (5)	0.9678 (2)	0.61730 (14)	0.0598 (7)
H15	1.127308	1.028796	0.650999	0.072*
C16	1.2391 (4)	0.9490 (2)	0.56820 (14)	0.0568 (7)
H16	1.363416	0.997684	0.567786	0.068*

antimicrobial [8]. The molecular structure of a compound determines its properties. Therefore, the investigation on the crystal structures of benzothiazoles has received wide attention [5, 9–11]. However, the crystal structure of naphthothiazole derivatives is less studied [12].

Single-crystal structure analysis reveals that the title compound crystallizes in the monoclinic space group $P2_1/n$. In the molecular structure (Figure), the dihedral angle between the almost planar naphtho[2,1-*d*]thiazole ring system (S1/N1/C1–C11) and the benzene ring of the 2-fluorophenyl group (C12–C17) is 2.36(1)°. Bond lengths and angles are all in the expected ranges [5, 11, 12]. The bond lengths of C–N is 1.305(3) and 1.364(3) Å, and C–S are 1.719(2) and 1.752(2) Å.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work was supported by the Hunan Provincial Natural Science Foundation of China (No. 2021JJ40010), and College Students Innovation and Entrepreneurship Training Program of Hunan Province General Project (No. cxcy2022011), Science and Technology Plan Project of Hengyang City (No. 202002042081).

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

References

1. Rigaku O. D. CrysAlis^{PRO}; Rigaku Oxford Diffraction Ltd: Yarnton, Oxfordshire, England, 2015.
2. Sheldrick G. M. *SHELXTL* – integrated space-group and crystal-structure determination. *Acta Crystallogr.* 2015, *A71*, 3–8.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Farrugia L. J. WinGX and Ortep for Windows: an update. *J. Appl. Crystallogr.* 2012, *45*, 849–854.
5. Zhu X., Yang Y., Xiao G., Song J., Liang Y., Den G. Double C–S bond formation *via* C–H bond functionalization: synthesis of benzothiazoles and naphtho[2,1-*d*]thiazoles from *N*-substituted arylamines and elemental sulfur. *Chem. Commun.* 2017, *53*, 11917–11920.
6. Weekes A. A., Westwell A. D. 2–Arylbenzothiazole as a privileged scaffold in drug discovery. *Curr. Med. Chem.* 2009, *16*, 2430–2440.
7. Sun Q., Wu R., Cai S., Lin Y., Sellers L., Sakamoto K., He B., Peterson B. R. Synthesis and biologicalevaluation of analogues of AKT (protein kinase B) inhibitor–IV. *J. Med. Chem.* 2011, *54*, 1126–1139.
8. Silva L. T., Azeredo J. B., Saba S., Rafique J., Bortoluzzi A. J., Braga A. L. Solvent- and metal-free chalcogenation of bicyclic arenes using I_2/DMSO as non-metallic catalytic system. *Eur. J. Org. Chem.* 2017, *2017*, 4740–4748.
9. Song Y., Hu L., Cheng Q., Chen Z., Su H., Liu H., Liu R., Zhu S., Zhu H. Benzothiazole derivatives with varied π-conjugation: synthesis, tunable solid-state emission, and application in single-component LEDs. *J. Mater. Chem. C* 2022, *10*, 6392–6401.
10. Wang Q., Tao Q., Dong H., Ni C., Xie X., Hu J. Fluorination triggers fluoroalkylation: nucleophilic perfluoro-*tert*-butylation with 1,1-dibromo-2,2-bis(trifluoromethyl)ethylene (DBBF) and CsF. *Angew. Chem., Int. Ed.* 2021, *60*, 27318–27323.
11. Vijayakumar S., Murugavel S., Selvakumarc R., Bakthadoss M. 2-(2–Nitrophenyl)-1,3-benzothiazole. *Acta Crystallogr.* 2012, *E68*, o2362.
12. Hosten E. C., Betz R. The crystal structure of 2-methyl-*α*-naphthothiazole, $C_{12}H_9NS$. *Z. Kristallogr. N. Cryst. Struct.* 2021, *236*, 483–485.