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STRUCTURE OF ORGANIC COMPOUNDS

Synthesis, Structural Characterization, and DFT Calculations of 3-Buthyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3*H*)-thione[1]

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Abstract—The title compound, $C_{21}H_{29}NS_2$, has been synthesized and its crystal structure has been determined from single crystal X-ray diffraction data. Crystals are monoclinic, a = 11.4923(8), b = 13.1842(7), c = 14.6583(8) Å, β = 109.983(6)°, sp. gr. $P2_1/c$, Z = 4. Mesityl and thiazole groups are in *cis* positions with respect to the cyclobutane ring. The cyclobutane ring is puckered, with a dihedral angle of 26.6(2)° between the two three-atom planes. The crystal structure involves one weak intermolecular C—H···S hydrogen-bond. The molecular geometry was also optimized using density functional theory (DFT/B3LYP) method with the 6-311G(d, p) basis set in ground state. Geometric parameters (bond lengths, bond angles and torsion angles) and vibrational assignments have been calculated theoretically and compared with the experimental data.

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INTRODUCTION

Organic compounds containing five-membered aromatic heterocyclic rings form a wide range of compounds in the nature and often play an important role in diverse biochemical processes. 1,3-Thiazole-2(3*H*)-thiones and their derivatives that widely investigated due to their biological activity, have been used in many research fields such as photography, agrochemistry and radiochemistry. They have nematocidal, insecticidal, antibacterial, antifungal, antiviral and antioxidant activity [1–3]. On the other hand, as a starting material, cyclobutanes are also used in various areas of chemistry [4].

In this article, the title thiazole derivative, 3-buthyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3*H*)-thione,has been investigated both experimentally and theoretically.

EXPERIMENTAL

Synthesis. Potassium acetate (9.8 g, 0.1 mol) was added in portions to a stirred solution of butylamine (7.3 g, 0.1 mol) in diethyl ether (50 ml) at 0°C. After stirring for 30 min, carbon disulfide (7.6 g, 0.1 mol) was added dropwise at 0–10°C over 1 h. The reaction mixture was stirred at 25–30°C for 18 h. The solid thus formed was collected by filtration, washed with diethyl ether (150 mL) and dried in air at 25–30°C. Potassium buthyldithiocarbamatesalt, [$C_4H_9NHC(=S)SK$], was obtained in 97% yield and was used without further purification (Scheme 1).

2-Chloro-1-(3-methyl-3-mesitylcyclobutyl)ethan-1-one (0.053 g, 0.02 mol) was added in portions to a stirred slurry containing the above potassium salt (5.62 g, 0.03 mol) in ethanol (50 mL). After stirring for 50 min the temperature had risen from 20 to 40°C. The stirred reaction mixture was heated at reflux (78–80°C) for 4 h and then allowed to cool. Stirring was maintained at 25–30°C for 24 h. After cooling to 5°C, water (60 mL) was added. The solid product *3*-butyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3H)-thione was collected by filtration, washed with water, recrystallized from ethanol and dried at 25–30°C (Scheme 2).

Characterization. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL 90-MHz spectrometer in $CDCl_3$. Elemental analyses were performed using a Thermo Flash2000 (CHNS) analyzer. Melting points was measured on a Stuart SMP40 Melting Point Apparatus and are uncorrected.

3-Butyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3H)-thione: white crystals (Yield: 85%),^{1}H NMR ($CDCl_3$, ppm): 1.07 (t, 3H, CH_3CH_2), 1.14–1.75 (m, 4H, CH_2), 1.63 (s, 3H, cyclobutane-CH_3), 2.2 (s, 6H, CH_3-mesitylene), 2.40–2.75 (m, 4H, CH_2 of cyclobutane), 3.33 (quint, 1H, CH of cyclobutane), 4.10 (t, 2H,NCH_2), 6.16 (s, 1H, =CH of thiazolethi-

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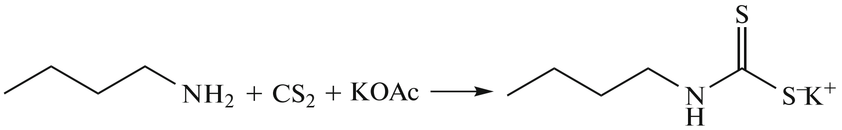
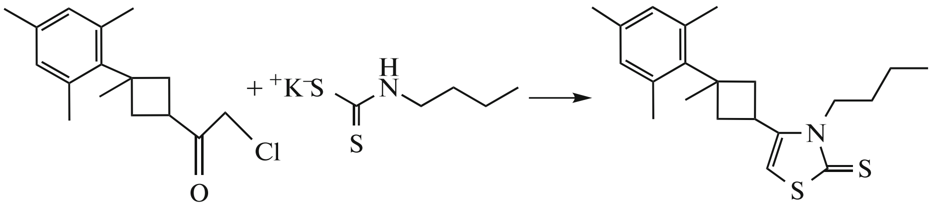


Scheme 1. Synthesis of potassium buthyldithiocarbamate.



Scheme 2. Synthesis of 3-butyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3H)-thione.

one ring), 6.77 (s, 2H, mesitylene aromatics). ^{13}C NMR ($CDCl_3$, ppm): 13.4, 20.1, 21.1, 24.5, 28.67, 29.3, 42.56, 40.88, 42.56, 47.18, 104.8, 130.5, 134.8, 147.3, 187.24. Anal. Calcd. for $C_{21}H_{29}NS_2$: C, 70.14; H, 8.13; N, 3.90; S, 17.83. Found: C, 70.25; H, 8.00; N, 3.85; S, 17.88%.

Table 1. Crystallographic characteristics and the X-ray-data collection and structure-refinement parameters for $C_{21}H_{29}NS_2$

System, sp. gr., Z	Monoclinic, $P2_1/c$, 4
a, b, c, Å	11.4923(8), 13.1842(7), 14.6583(8)
β, deg	109.983(6)
V, Å^3	2087.3(2)
D_x, g cm^{-3}	1.144
Radiation, λ, Å	MoK_α, 0.71073
μ, mm^{-1}	0.257
T, K	293(2)
Sample size, mm	0.5644 × 0.4676 × 0.3955
Diffractometer	Agilent Diffraction Xcalibur, Eos CCD
Scan mode	ω
Absorption correction, $T_{\min}$, $T_{\max}$	Analytical, 0.908, 0.926
$\theta_{\max}$, deg	26.372
h, k, l ranges	$-14 \leqslant h \leqslant 12$, $-9 \leqslant k \leqslant 16$, $-18 \leqslant l \leqslant 16$
Number of reflections: measured/unique ($N1$), R_{int}/with $I > 2\sigma(I)$ ($N2$)	8596/4264, 0.0189/2953
Refinement method	Least squares on F^2
Number of refined parameters	222
$R1/wR2$ relative to $N1$	0.0817/0.1626
$R1/wR2$ relative to $N2$	0.0541/0.1430
S	1.033
$\Delta\rho_{\max}/\Delta\rho_{\min}$, e/Å^3	0.42/–0.32
Programs	CrysAlis$^{\text{Pro}}$ [5], OLEX2 [6], SHELX97 [7]

X-ray crystal structure determination: The structure of the title compound is determined by single crystal X-ray diffraction. The summary of the crystal data, experimental details and refinement results are listed in Table 1. Crystal structure was solved by the direct method. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were treated as riding atoms. Geometrical calculations were performed using PLATON [8]. The figures were made using ORTEP [9] and PLATON [8].

CCDC 1057497 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Computational details: All the calculations were performed using Gaussian 09W program package [10]. For modeling, the initial guess of the compound was obtained from the X-ray coordinates and the structure was optimized by Density Functional Theory (DFT)/B3LYP methods [11–13] with 6-311G(d, p) [14] as basis set. Vibrational frequencies for optimized molecular structures have been calculated. The vibrational frequencies for DFT(B3LYP)/6-311G(d, p) are scaled by 0.9669 [15].

RESULTS AND DISCUSSION

The molecular geometry. The molecule (Fig. 1) contains three rings, namely a cyclobutane ring (C10–C13), a mesityl ring (C1–C9) and a thiazole ring (C15–C17/N1/S1). The mesityl and thiazole groups are in *cis* positions with respect to the cyclobutane ring. The steric interaction between the substituent groups at the cyclobutane ring causes the significant deviation of this ring from planarity. Values for the puckering of cyclobutane have been reported as 23.5–24.3° [16, 17]. In the title molecule, the cyclobutane ring is distinctly puckered, with a dihedral angle between C11/C12/C13 and C13/C10/C11 planes of 26.6(2)°.

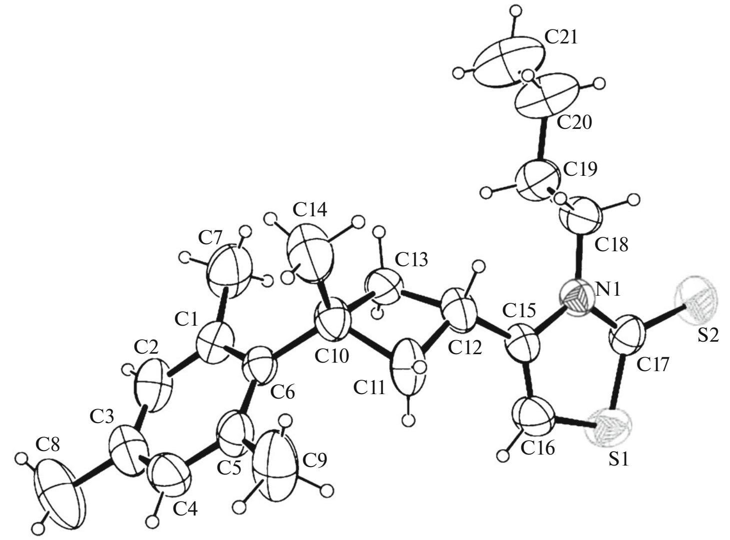


Fig. 1. The molecular structure and atom-numbering scheme for the title compound. Displacement ellipsoids are shown at the 50% probability level.

The bond distances and angles in the cyclobutane ring are in good agreement with the literature values [18–21].

The thiazolethione system is essentially planar and makes a dihedral angle of 78.99(1)° with the mean plane of the phenyl ring. This value is slightly less than dihedral angles reported for other structures including a phenyl–thiazole ring system [3, 22]. The C16–S1–C17 bond angle of 91.93(13)° shows that the heterocyclic ring is distorted from a regular pentagon. The two endocyclic heteroatoms, N1 and S1, form single bonds with the adjacent C atoms. The N1–C17 bond length [1.353(3) Å] indicates partial delocalization along this bond. NBO analysis verifies this inference [23–25]. Hybridization of N1 atom is obtained as $sp^{3.546}$. The reason for residual electronic population of *p*-orbitals relative to sp^3 hybridization is mesomeric effect between S2 and N1 atoms leading to a delocalized path over the atoms S2, C17 and N1. S1–C16 and S1–C17 bonds are shorter than the reported mean value for S-Csp^2 single bond lengths (1.76 Å) [26]. These values are comparable with those in related structures [27, 28]. Likewise, the C2–S2 bond length is close to the values reported in the literature [29, 30].

The value of the N1–C18–C19–C20 torsion angle [−177.0(2)°] implies a *trans* conformation for the butyl chain. The mean plane of the *n*-butyl chain (C18–C21) is nearly perpendicular to the benzene ring as indicated by the dihedral angle between them of 88.76(16)°.

Table 2. Hydrogen-bond geometry

D–H···*A*	*D*–H, Å	H···*A*, Å	*D*···*A*, Å	*D*–H···*A*, deg
C16–H16···S2^i	0.93	2.87	3.706(3)	150
C18–H18*A*···S2	0.97	2.74	3.127(3)	105

Symmetry code: (i) *x*, 1/2 − *y*, 1/2 + *z*.

The compound contains intra- and intermolecular C–H···S=C interactions (Table 2): C18–H18A···S2 interaction generates an S(5) ring motif [31] and C16–H16···S2 (*x*, 1/2 − *y*, 1/2 + *z*) interaction [32, 33] links the molecules into an infinite one-dimensional chain along the [001] direction (Fig. 2).

The molecular structure of the title compound was also calculated theoretically. The starting geometry was that obtained from the X-ray structure determination and the molecular geometry was optimized using Density Functional Theory (DFT/B3LYP) method with the 6-311G(*d*, *p*) basis sets in ground state. Some optimized parameters (bond lengths, bond angles and dihedral angles) are compared with the experimental data (Table 3).

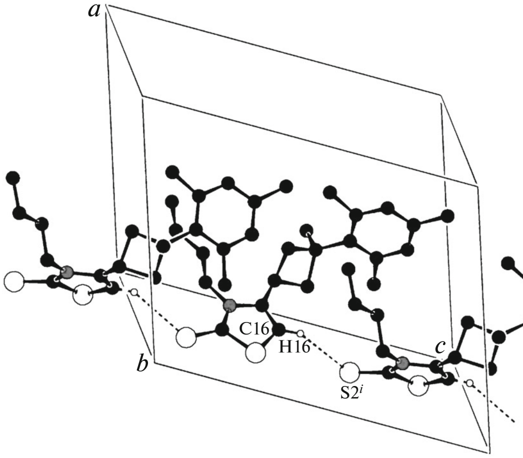


Fig. 2. Packing diagram of the title compound showing C–H···S hydrogen bonds which forms an infinite chain along the [001] direction. For clarity, only H atoms involved in hydrogen bonding have been included.

Table 3. Experimental and optimized geometrical parameters of the title compound

Geometric parameters	Experimental (X-ray)	Calculated B3LYP/6-311G(*d*,*p*)	Geometric parameters	Experimental (X-ray)	Calculated B3LYP/6-311G(*d*,*p*)
Bond lengths, Å					
S1–C16	1.714(3)	1.7452	C6–C10	1.524(3)	1.5333
S1–C17	1.713(3)	1.7610	C10–C11	1.555(3)	1.5724
S2–C17	1.666(2)	1.6672	C10–C13	1.553(3)	1.5710
N1–C15	1.405(3)	1.4064	C10–C14	1.533(4)	1.5413
N1–C17	1.353(3)	1.3741	C11–C12	1.527(3)	1.5438
N1–C18	1.460(3)	1.4713	C12–C13	1.544(3)	1.5549
C1–C2	1.387(4)	1.3976	C12–C15	1.483(3)	1.4968
C1–C6	1.395(3)	1.4151	C15–C16	1.327(4)	1.3495
C1–C7	1.510(4)	1.5170	C18–C19	1.504(4)	1.5322
C3–C8	1.514(4)	1.5091	C20–C21	1.471(6)	1.5312
C5–C9	1.508(4)	1.5171			
Bond angles, deg					
C16–S1–C17	91.93(13)	91.759	C11–C12–C13	87.53(17)	87.777
C15–N1–C17	115.16(19)	115.876	C11–C12–C15	117.8(2)	118.744
C15–N1–C18	123.96(19)	123.972	C13–C12–C15	117.8(2)	120.684
C17–N1–C18	120.88(19)	120.151	C10–C13–C12	89.63(18)	89.47
C6–C10–C11	117.28(19)	117.801	N1–C15–C16	111.4(2)	112.24
C6–C10–C13	118.84(19)	118.156	S1–C16–C15	112.39(19)	111.835
C6–C10–C14	109.73(19)	110.217	S1–C17–S2	122.86(15)	123.972
C11–C10–C13	86.21(17)	86.220	S1–C17–N1	109.16(17)	108.280
C11–C10–C14	111.6(2)	111.406	S2–C17–N1	127.95 (19)	127.745
C13–C10–C14	111.5(2)	111.136	N1–C18–C19	112.9 (2)	113.257
C10–C11–C12	90.21(18)	89.822			
Torsion angles, deg					
C15–N1–C18–C19	−92.2(3)	−96.91	C6–C10–C11–C12	139.7(2)	139.34
C18–N1–C15–C16	−178.9(2)	178.95	C13–C12–C15–N1	89.3(3)	75.6
C17–1–C18–C19	88.2(3)	82.7	C12–C15–C16–S1	179.3(2)	−177.47
C5–C6–C10–C13	142.4(2)	142.97	N1–C18–C19–C20	−177.0(2)	−178.5
C5–C6–C10–C11	40.9(3)	41.57	C18–C19–C20–C21	179.3(3)	179.44

Theoretical values were correlated with corresponding experimental values, and the correlation coefficient were 0.98053 for bond lengths, 0.99755 for bond angles, 0.991 for torsion angles (Fig. 3).

Vibrational spectra. IR spectra (cm^{-1}) were recorded on a Perkin Elmer FT-IR Spectrum 100 spectrometer with ATR unit. Theoretical spectra were calculated by B3LYP/6-311G(d, p) methods for opti-

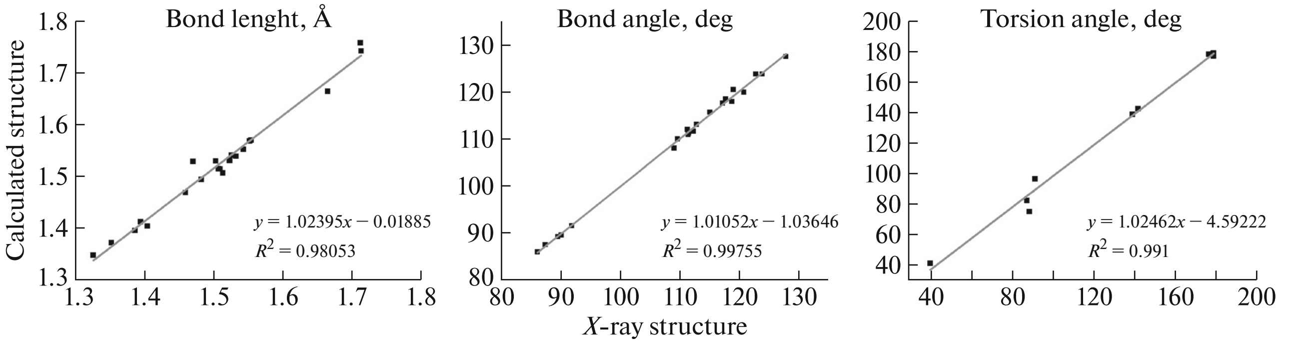


Fig. 3. Correlation graphics between the experimental and theoretical geometric parameters of the title compound.

Table 4. Comparison of the observed and calculated vibrational spectra of the title compound

Vibrational mode	Experimental IR, cm^{-1}	Calculated [B3LYP] 6-311G(d,p)	Vibrational mode	Experimental IR, cm^{-1}	Calculated [B3LYP] 6-311G(d,p)
		scaled frequency, cm^{-1}			scaled frequency, cm^{-1}
νC–H$_{\mathrm{thiazole}}$	3090.90	3158	umC–H$_{\mathrm{3phenyl}}$	1369.72	1365
ν_sC–H$_{\mathrm{phenyl}}$	3076.92	3044	umC–H$_{\mathrm{3cyclo}}$	–	1364
ν_{as}C–H$_{\mathrm{phenyl}}$	–	3041	umC–H$_{\mathrm{3butyl}}$	1353.70	1362
ν_{as}C–H$_{2cyclo}$	2954.24	3020	γC–H$_{\mathrm{cyclo}}$	1344.06	1314
ν_{as}C–H$_{2cyclo}$	2930.06	3018	ωC–H$_{\mathrm{2butyl}}$	1294.40	1299
ν_{as}C–H$_{3\mathrm{mesitylene}}$	–	2991	δC–H$_{\mathrm{2butyl}}$	1275.32	1271
ν_{as}C–H$_{3cyclo}$	–	2987	Θ_{phenyl}	–	1268
ν_{as}C–H$_{3}$	–	2987	ωC–H$_{\mathrm{2cyclo}}$	1260.50	1267
ν_sC–H$_{2cyclo}$	–	2964	γC–H$_{\mathrm{thiazole}}$	1208.88	1193
ν_sC–H$_{2cyclo}$	–	2958	γC–H$_{\mathrm{phenyl}}$	1182.65	1172
νC–H$_{cyclo}$	2867.13	2939	νC–N	1153.80	1169
ν_sC–H$_{\mathrm{3mesitylene}}$	–	2928	νC=S	1126.65	1151
ν_sC–H$_{3cyclo}$	–	2925	γC–H$_{\mathrm{2butyl}}$	1136.80	1130
ν_sC–H$_3$	–	2923	δC–H$_{\mathrm{2cyclo}}$	–	1122
νC=C$_{\mathrm{phenyl}}$	1611.07	1595	γC–H$_{\mathrm{2cyclo}}$	1070.97	1110
νC=C$_{\mathrm{thiazole}}$	1569.54	1566	γC–H$_{\mathrm{cyclo}}$	1014.48	980
νC=C$_{\mathrm{phenyl}}$	–	1551	Θ_{cyclo}	955.84	963
αC–H$_3$	1484.30	1455	ΓC–H$_{\mathrm{phenyl}}$	919.13	866
αC–H$_{2cyclo}$	1464.70	1454	ΓC–H$_{\mathrm{phenyl}}$	857.92	840
αC–H$_{\mathrm{3phenyl}}$	1455.10	1453	νC–S	843.87	816
αC–H$_{\mathrm{2butyl}}$	1439.39	1449	ΓC–H$_{\mathrm{thiazole}}$	731.72	703
αC–H$_{3cyclo}$	1427.16	1447			

Vibrational modes: ν_s, symmetric stretching; ν_{as}, asymmetric stretching; α, scissoring; γ, rocking; ω, wagging; δ, twisting; Θ, ring breathing; Γ, out-of-plane bending; *um,* umbrella.

mized geometries. Some vibrational modes assigned by Gauss View software [34] are given in Table 4 with their corresponding experimental values. Comparison of the calculated vibrational frequencies to their experimental data gives correlation value (R^2) of 0.99868 (Fig. 4). So, calculations have a good correlation with experimental X-ray and IR data.

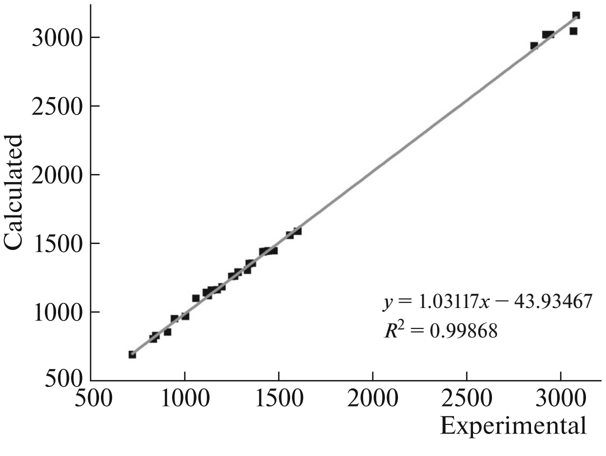


Fig. 4. Correlation graphic between the experimental and theoretical vibration frequencies of the title compound (cm^{-1}).

The aromatic structure shows the presence of vibrations in the range 3100–3000 cm^{-1} characteristic for C–H stretching [35–37]. The C–H symmetric stretching was recorded at 3076.92 cm^{-1} in FT-IR spectrum, also calculated as 3044 cm^{-1} B3LYP/6-311G(d, p) level.

There are many cyclobutane ring vibrations. The asymmetric stretching C–H$_2$ is observed at 2954.24 and 2930.06 cm^{-1} in FT-IR spectrum and also these vibrations are calculated at 3020 and 3018 cm^{-1} for B3LYP. There are no peaks observed in FT-IR spectrum for C–H$_2$ symmetric stretching vibrations but these vibrations are calculated at 2964 and 2958 cm^{-1}. The scissoring C–H$_2$, rocking C–H, twisting C–H$_2$ and rocking C–H$_2$ vibrations are observed at 1464.70, 1344.06, 1260.50, and 1070.97 cm^{-1} in FT-IR spectrum for cyclobutane ring.

For the thiazole ring, the C—H symmetric stretching vibration has only one peak at 3090.90 cm^{-1} at the left part of the spectrum. The C—H out-of-plane bending vibration of thiazole ringis determined at 731.72 cm^{-1} in FT-IR spectrumand its corresponding calculated frequency is 703 cm^{-1} using B3LYP/6-311G(*d*, *p*).

CONCLUSIONS

3-Buthyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3*H*)-thione was synthesized and its molecular and crystal structure was determined by single crystal X-ray diffraction. The spectroscopic properties of the compound were examined by FT-IR , ^{1}H NMR and ^{13}C NMR techniques. To support the solid state structure, the geometric parameters and vibrational frequencies of the title compound have been calculated using the density functional theory DFT/B3LYP method with the 6-311G(*d*, *p*) basis set. Comparison of theoretical data with the experimental results shows no significant differences, even though the experimental results belong to solid phase and theoretical calculations belong to gaseous phase.

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REFERENCES

1. M. Ahmedzade, C. Kirilmis, A. Cukurovali, et al., S. Afr. J. Chem. **56**, 21 (2003).
2. J. Safaei-Ghomi, F. Salimi, and A. Ramazani, J. Chem. Sci. **125**, 1087 (2013)
3. C. Kırılmış, M. Koca, C. Arıcı, et al., Acta Crystallogr. E **61**, o555 (2005).
4. F. Yakuphanoglu, A. Cukurovali, and I. Yilmaz, Opt. Mater. **27**, 1363 (2005).
5. *CrysAlis Pro Software System, Version 1.171.35.11* (Agilent Technologies UK, 2011).
6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, et al., J. Appl. Crystallogr. **42**, 339 (2009).
7. G. M. Sheldrick, Acta Crystallogr. A **64**, 112 (2008).
8. A. L. Spek, J. Appl. Crystallogr. **36**, 7 (2003).
9. L. J. Farrugia, J. Appl. Crystallogr. **30**, 565 (1997).
10. M. J. Frisch, G. W. Trucks, H. B. Schlegel, et al., *Gaussian 09, revision **B.01*** (Gaussian, Wallingford, 2010).
11. A. D. Becke, Phys. Rev. A **38**, 3098 (1988).
12. A. D. Becke, J. Chem. Phys. **98**, 5648 (1993).
13. C. Lee, W. Yang, and R. D. Parr, Phys. Rev. B. **37**, 785 (1998).
14. G. A. Petersson, A. Bennett, T. G. Tensfeldt, et al., J. Chem. Phys. **89,** 2193 (1988).
15. K. K. Irikura, R. D. Johnson, III, and R. N. Kacker, J. Phys. Chem. A **109**, 8430 (2005).
16. D. C. Swenson, M. Yamamoto, and D. J. Burton, Acta Crystallogr. C **53**, 1445 (1997).
17. F. H. Allen, Acta Crystallogr. **B40**, 64 (1984).
18. M. Dinçer, N. Özdemir, A. Çukurovalı, et al., Acta Crystallogr. E **60**, o1523 (2004).
19. F. Sen, M. Dinçer, A. Çukurovali, et al., Acta Crystallogr. E **67**, o958 (2011).
20. F. Şen, M. Dinçer and A. Cukurovali, J. Mol. Struct. **1076**, 1 (2014).
21. M. Koca, C. Kirilmiş, and C. Arici, Acta Crystallogr. E **66**, o523 (2010).
22. C. Kırılmış, M. Koca, C. Arıcı, et al., Acta Crystallogr. E **61**, o1176 (2005).
23. J. P. Foster and F. Weinhold, J. Am. Chem. Soc. **102,** 7211 (1980).
24. A. E. Reed and F. Weinhold, J. Chem. Phys. **78**, 4066 (1983).
25. A. E. Reed, R. B. Weinstock and F. Weinhold, J. Chem. Phys. **83**, 735 (1985).
26. F. H. Allen, O. Kennard, D. G. Watson, et al., J. Chem. Soc. Perkin Trans. **2**, S1 (1987).
27. J. Hartung, N. Schneiders, and U. Bergsträsser, Acta Crystallogr. E **62**, o4713 (2006).
28. J. Hartung, N. Schneiders, and U. Bergsträsser, Acta Crystallogr. E **61**, o421 (2005).
29. J. Hartung, M. Schwarz, E. F. Paulus, et al., Acta Crystallogr. C **62**, o386 (2006).
30. J. Hartung, S. Altermann, I. Svoboda, et al., Acta Crystallogr. E **61**, o1738 (2005).
31. J. Bernstein, R. E. Davis, L. Shimoni, et al., Angew. Chem. Int. Ed. Engl., **34**, 1555 (1995).
32. T. Steiner, Crystallogr. Rev. **6**, 1 (1996).
33. J. Hartung, M. Schwarz, I. Svoboda, et al., Acta Crystallogr. C **59**, o682 (2003).
34. R. Dennington, II, T. Keith, and J, Millam, *GaussView, Version 4.1.2* (SemichemInc, Shawnee Mission, KS, 2007).
35. G. Socrates, *Infrared Characteristic Group Frequencies* (Wiley, New York, 1980).
36. F. R. Dollish, W. G. Fateley, and F. F. Bentley, *Characteristic Raman Frequencies of Organic Compounds* (Wiley, New York, 1997).
37. G. Varsanyi, *Vibrational Spectra of Benzene Derivatives* (Academic, NewYork, 1969).