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CRYSTALLOGRAPHIC AND THEORETICAL STUDIES OF
1-(1-NAPHTHYL)-2-THIOUREA WITH INTERMOLECULAR N—H...S HETEROATOM
INTERACTION AND N—H... π INTERACTION

M.A. AlDamen¹, M. Sinnokrot²¹Department of Chemistry, Faculty of Science, The University of Jordan, Amman, Jordan

E-mail: maldamen@ju.edu.jo

²Department of Chemistry, Arts and Sciences Program, The Petroleum Institute, Abu Dhabi 2533 UAE

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A single crystal X-ray diffraction study of 1-(1-naphthyl)-2-thiourea (**1**) C₁₁H₁₀N₂S indicates crystallization in the monoclinic space group *C2/c*, *Z* = 8, with unit cell parameters *a* = 15.3864(14) Å, *b* = 7.6090(7) Å, *c* = 17.0836(16) Å, β = 91.7420(30)°. In the crystal structure, two components of **1** are connected via intermolecular NH...S hydrogen bonds (the N...S distance of 3.371 Å). In **1** there is an NH... π interaction (with the N... π distance of 3.804 Å and a possible N—H... π distance of 3.196 Å). The calculations of **1** at the B3LYP/*cc-pVTZ*, RHF/*cc-pVTZ*, RIMP2/*cc-pVDZ*, and RIMP2/*cc-pVTZ* levels of theory can almost reproduce the X-ray geometry. In addition, the binding energies of a dimer of **1** calculated by RIMP2 using the *cc-pVDZ* and *cc-pVTZ* corrected BSSE basis sets are –36.1 kJ/mol and –41.7 kJ/mol. The results suggest that complex **1** is significantly important for the attractive intermolecular interaction in **1**.

Keywords: 1-(1-naphthyl)-2-thiourea, S...H—N hydrogen bond, interaction energy, *ab initio*, RIMP2, B3LYP.

INTRODUCTION

Besides the well-known classical hydrogen bonding also new types of interactions have recently been documented. Examples of such interactions include π — π stacking, cation- π , anion- π interactions and halogen...halogen interactions to name a few. Further, the hydrogen bonding definition has been expanded to include heteroatoms such as halogens, chalcogens, and pnictogens as well as carbon itself. Among all these interactions, only few articles with clear statistics have recently been published considering sulfur S...H—(N,O) interactions [1].

Previous publications show that sulfur is not capable of being a hydrogen bond acceptor and this leads to scarcity of data. Recent studies have showed that this idea is not correct and sulfur may act as an acceptor. These interactions are important in modulating the high-grade structures and functions of many proteins, and much effort is needed to be done in order to estimate these values and therefore to extract information about their molecular dynamic behavior and parameters [2].

In the past decade, several intermolecular S...H—N hydrogen bonding patterns had been reported [3—5]. A research survey of such interactions shows that before 2001 the reported information about S...H—N or S—H...N was, at best, scattered and unclear. In the time when weak interactions such as halogen...O/N became a pivotal area of research, the interactions such as S...N hydrogen bonds remained in its infancy. Allen was the first to notice and report this S...H—N interaction by analyzing many systems in the database [6]. Afterwards a study which could be considered the turning point in

the literature for these interactions came to confirm it by using trimercaptotriazine as a sulfur hydrogen receptor. It was found that the S...N distances in this compound and other amines ranges 3.3—3.5 Å [3]. However, that study did not contain any theoretical details about the energy values of such interactions.

A benchmark detailed theoretical study about sulfur-containing hydrogen bonds suggests that sulfur is as good as oxygen in its ability of making hydrogen bond framework systems [2, 7]. The enhanced dispersion in S-containing systems compensates for the loss in the electrostatic contribution, and that the bond is dominated by the dipole-dipole interaction. Also, by observing the potential curve it was found to be flat even at an S...H distance of 3.0 Å. Finally, in a dimethylthiocarbonyl-methanol complex system, at the RIMP2 level of theory the hydrogen bond to disulfide has an energy of -22.3 kJ/mol at a distance of ~2.42 Å and an angle = 98°. The directionality in this interaction was previously reported in other systems such as H₂CS...HF with its energy calculated at the MP4/6-311++G(*d,p*) level to be -18.1 kJ/mol [8, 9].

Walters et al. studied the S...amine hydrogen bonding in xanthate without presenting any energy values or performing any calculation [10]. The hydrogen bond distance is large with nitrogen...sulfur separated at a distance of 3.567 Å.

Recently, Biswal et al. published a detailed comparative study of hydrogen-bonding interactions between *p*-cresol and the H₂S/H₂O systems [11]. They showed that both H₂O and H₂S form O—H...O/S σ -type hydrogen bonded complexes. They confirmed that O—H...S is weaker (with the main component being dispersion energy) than O—H...O, which is expected in view of their electronegativities. Also, Biswal and Wategaonkar studied other weaker (O, N, C)—H...S and S—H... π hydrogen bonds using computational methods as well as FTIR data [12]. They concluded at the MP2/*aug-cc-pVDZ* and *aug-cc-pVTZ* levels of theory (including the BSSE and ZPE corrections) that the S—H... π interaction is stronger than that with X—H... π (X = C, N, and O) and came with a new definition of hydrogen bonds: *the dispersion-stabilized hydrogen bonds*.

The above survey shows that the work in this field is in its infancy and that the need to obtain information on such interactions is necessary as it affects many force fields, and accordingly completes another part of the non-covalent puzzle. For this purpose, we studied 1-(1-naphthyl)-2-thiourea (**1**) as it contains two types of aminic moieties (primary and secondary amines) and the donating sulfonyl group.

In this article, we report the molecular and crystal structure, and the calculation results of **1**, which may give a hint to the energy values in sulfur...amine interactions.

EXPERIMENTAL

Preparation. All chemicals were commercially purchased and used without further purification. Crystals of the title compound were obtained since an attempt to react KMnO₄ with **1** failed.

X-ray crystallographic measurements. The frame data were collected at room temperature on a Bruker diffractometer equipped with an APEX II DUO detector using MoK radiation ($\lambda = 0.71073$ Å) at liquid nitrogen temperature. The frame data were acquired with the SMART software [13]. The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm [14]. The integration of the data to a maximum θ angle of 25.67° (0.82 Å resolution) using a monoclinic unit cell yielded a total of 7052 reflections out of which 1900 were independent (average redundancy 3.712, completeness = 99.7 %, $R_{\text{int}} = 2.53$ %), out of which 1594 (83.89 %) were greater than $2\sigma(F^2)$. The final cell constants are based on the refinement of the XYZ-centroids of 3194 reflections with $4.771 < 2\theta < 52.04^\circ$. Data were corrected for absorption effects using the numerical method (SADABS). The ratio of minimum to maximum apparent transmission was 0.840.

The structure was solved and refined using the Bruker SHELXTL Software Package [15]. The final anisotropic full-matrix least-squares refinement on F^2 with 127 variables converged at $R_1 = 3.08$ % for the observed data and $wR_2 = 7.93$ % for all data. The goodness-of-fit was 1.067. The largest peak in the final difference electron density synthesis was $0.341 \text{ e}/\text{Å}^{-3}$ and the largest hole

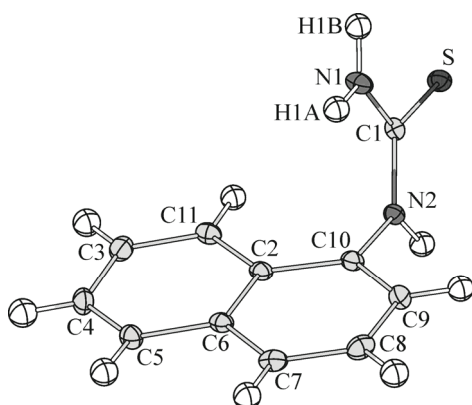


Fig. 1. Thermal ellipsoid (30 %) of the asymmetric unit of **1**

$-0.199 \text{ e}/\text{\AA}^{-3}$ with an RMS deviation of $0.044 \text{ e}/\text{\AA}^{-3}$. Based on the final model, the calculated density was $1.344 \text{ g}/\text{cm}^3$ and $F(000) = 848 \text{ e}^-$.

Hydrogen atoms were positioned and constrained with U_{eq} 1.2 times those of the riding atoms. The asymmetric unit with anisotropic thermal ellipsoids at 30 % probability is shown in Fig. 1. Final graphical parameters were obtained using the CrystalMaker 6.1® graphics program (licensed version) [16]. Crystal data and structure refinement details are summarized in Table 1. Table 2 shows the final fractional

atomic coordinates and isotropic displacement parameters.

Computational details. The Qchem program suite [17] was used for the *ab initio* molecular orbital calculations to evaluate total interaction energies. The geometrical parameters of all complexes and related free monomers were fully optimized at the RIMP2 (core frozen), B3LYP and RHF/*cc-pVTZ* levels of theory. The interaction energies were calculated between atoms in a dimer as obtained by X-ray crystallography without any further optimizations. The interaction energy was calculated at RIMP2/*cc-pVDZ* and *cc-pVTZ* levels. The basis set superposition error (BSSE) was corrected only at the RIMP2 level of theory.

Table 1

Crystal data and structure refinement for **1**

Empirical formula	$\text{C}_{11}\text{H}_{10}\text{N}_2\text{S}$
Formula weight	202.27
Temperature, K	100(2)
Wavelength, \AA	0.71073
Crystal system, mm	$0.13 \times 0.14 \times 0.47$
Space group	<i>C2/c</i>
Unit cell dimensions <i>a</i> , <i>b</i> , <i>c</i> , \AA ; β , deg.	15.3864(14), 7.6090(7), 17.0836(16); 91.742(3)
Volume, \AA^3	1999.1(3)
<i>Z</i>	8
Density (calculated), Mg/m^3	1.344
Absorption coefficient, mm^{-1}	0.282
$F(000)$	848
Crystal size, mm	$0.13 \times 0.14 \times 0.47$
θ range for data collection, deg.	2.39–25.67
Index ranges	$-18 \leq h \leq 18$, $-9 \leq k \leq 8$, $-20 \leq l \leq 18$
Reflections collected	7052
Independent reflections	1900 [$R_{\text{int}} = 0.0253$]
Completeness to $\theta = 25.67^\circ$	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1900 / 0 / 127
Goodness-of-fit on F^2	1.067
Final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0308$, $wR_2 = 0.0740$
<i>R</i> indices (all data)	$R_1 = 0.0413$, $wR_2 = 0.0793$
Largest diff. peak and hole, $\text{e}/\text{\AA}^{-3}$	0.341 and -0.199

Table 2

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S	0.13725(3)	0.07040(5)	0.47821(2)	0.02159(13)
N2	0.15446(8)	0.35352(18)	0.56725(7)	0.0215(3)
H2A	0.2048	0.3645	0.5446	0.026*
N1	0.02395(8)	0.21163(19)	0.57374(8)	0.0237(3)
H1A	0.0074	0.2911	0.6077	0.028*
H1B	-0.0116	0.126	0.5596	0.028*
C4	0.16358(11)	0.3474(3)	0.86662(9)	0.0276(4)
H4	0.1727	0.3197	0.9205	0.033*
C5	0.13943(11)	0.5125(2)	0.84524(9)	0.0255(4)
H5	0.1305	0.5984	0.8845	0.031*
C6	0.12721(9)	0.5593(2)	0.76503(9)	0.0199(3)
C11	0.14183(9)	0.4282(2)	0.70718(9)	0.0189(3)
C10	0.13381(10)	0.4792(2)	0.62675(9)	0.0203(4)
C1	0.10264(10)	0.2209(2)	0.54392(8)	0.0195(3)
C7	0.10514(10)	0.7318(2)	0.74155(10)	0.0257(4)
H11	0.0961	0.8194	0.7801	0.031*
C8	0.09659(11)	0.7744(2)	0.66370(10)	0.0277(4)
H8	0.0807	0.8904	0.6486	0.033*
C9	0.11140(10)	0.6462(2)	0.60617(9)	0.0245(4)
H9	0.1057	0.6767	0.5523	0.029*
C3	0.17520(10)	0.2170(2)	0.80952(9)	0.0257(4)
H3	0.1902	0.1008	0.8252	0.031*
C2	0.16505(10)	0.2559(2)	0.73165(9)	0.0220(4)
H2	0.1736	0.167	0.6937	0.026*

RESULTS AND DISCUSSION

Molecular and crystal structure by X-ray diffraction. The molecular structure of **1** is shown in Fig. 1. Selected bond distances and angles are listed in Table 3. The crystal of **1** crystallizes in the $C2/c$ space group. Each molecule is located on an inversion center and is therefore perfectly centrosymmetric. The bond distances and angles are within normal ranges of other naphthalene and thiourea derivatives [18, 19].

An analysis of the crystal structure of **1** shows that the asymmetric unit consists of only one moiety. The view down the z axis of the xy plane is shown in Fig. 2, *a* and down the a axis of the yz plane in Fig. 2, *b*. It is possible to see *zigzag* interactions in the yz plane along the y axis as well as along the z axis (Fig. 2, *b*). Fig. 2, *c* shows intramolecular interactions of the $N-H\cdots\pi$ and $C-H\cdots\pi$ type as well as an intermolecular hydrogen bond of the $N-H\cdots S$ type in the dimer unit (bottom view). Apart from the intramolecular $N1-H2A\cdots\pi$ interaction at a distance of 3.196 \AA there are structural features to be evaluated in the tail-like arrangement with angles $C2-N2-C1$ (124.688°), $N2-C1-N1$ (117.838°), $C1-N1-H2A$ (120.001°), and $N1-H2A$ -centroide (128.330°). The other two intermolecular interactions evaluated are $C-H\cdots\pi$ (2.941 \AA) and the intermolecular hydrogen bonding to S from NH at distances $S\cdots H$ (2.523 \AA) and $S\cdots N$ (3.371 \AA) showed in the Fig. 3, *c*. Although this distance is not a new record in $S\cdots N$ reported hydrogen bonds, it is still much less than the average distances in the reported structures (in a survey of the Cambridge Structural Database, $S\cdots H$ of 2.75 \AA

Table 3

Selected bond distances (Å) and angles for 1 determined by X-ray diffraction and theoretical HF, B3LYP and RIMP2 calculations.

Last row is the energy calculated at each level in kJ/mol

Bond distances	X-ray	HF	B3LYP	RIMP2
S—C1	1.7006(16)	1.683	1.677	1.662
N2—C1	1.339(2)	1.341	1.365	1.365
N2—C10	1.438(2)	1.424	1.427	1.416
N2—H2A	0.88	0.992	1.007	1.008
N1—C1	1.330(2)	1.33	1.349	1.352
N1—H1A	0.88	0.991	1.005	1.006
N1—H1B	0.88	0.989	1.003	1.003
C4—C5	1.357(3)	1.354	1.369	1.376
C4—C3	1.407(2)	1.412	1.411	1.411
C4—H4	0.95	1.073	1.082	1.081
C5—C6	1.423(2)	1.417	1.417	1.376
C5—H5	0.95	1.073	1.083	1.081
C6—C7	1.411(2)	1.416	1.415	1.415
C6—C11	1.427(2)	1.406	1.429	1.431
Bond angles	X-ray	HF	B3LYP	RIMP2
C1—N2—C10	124.69(13)	126.595	127.144	125.659
C1—N2—H2A	117.7	114.315	113.43	113.812
C10—N2—H2A	117.7	118.785	118.677	119.691
C1—N1—H1A	120	122.419	122.549	121.439
C1—N1—H1B	120	117.689	117.392	116.5
H1A—N1—H1B	120	119.891	119.731	119.703
C11—C10—N2	118.95(14)	119.675	120.204	119.626
N1—C1—N2	117.84(14)	117.299	116.369	115.358
N1—C1—S	121.60(12)	121.84	122.348	123.068
N2—C1—S	120.56(12)	120.861	121.255	121.557
Torsion angles	X-ray	HF	B3LYP	RIMP2
C10—N2—C1—N1	5.0(2)	4.705	3.573	3.288
C2—C11—C10—N2	3.3(2)	1.257	0.589	1.365
C6—C11—C10—N2	175.42(13)	178.718	179.739	179.313
C1—N2—C10—C9	106.24(18)	88.948	106.405	110.777
C1—N2—C10—C11	77.08(19)	92.231	75.646	70.715
C10—N2—C1—S	175.04(12)	175.161	176.857	178.132
N2—C10—C9—C8	175.74(14)	179.076	178.557	179.166
C7—C8—C9—C10	0.3(2)	0.382	0.873	1.097
Energy, kJ/mol	—	−929.0	−933.1	−931.3

and S...N of 3.58 Å) [5]. This hydrogen bonding is important as stated in a recent study of enzyme structures. Another interaction of the electrostatic nature that is worthy of mentioning is NH... π (3.166 Å). It is important to notice that the consideration of the hydrogen...S interaction is not possible because no neutron diffraction data is available and we depend on the model system in SHELXTL as well as the heavy atoms at N...S distances.

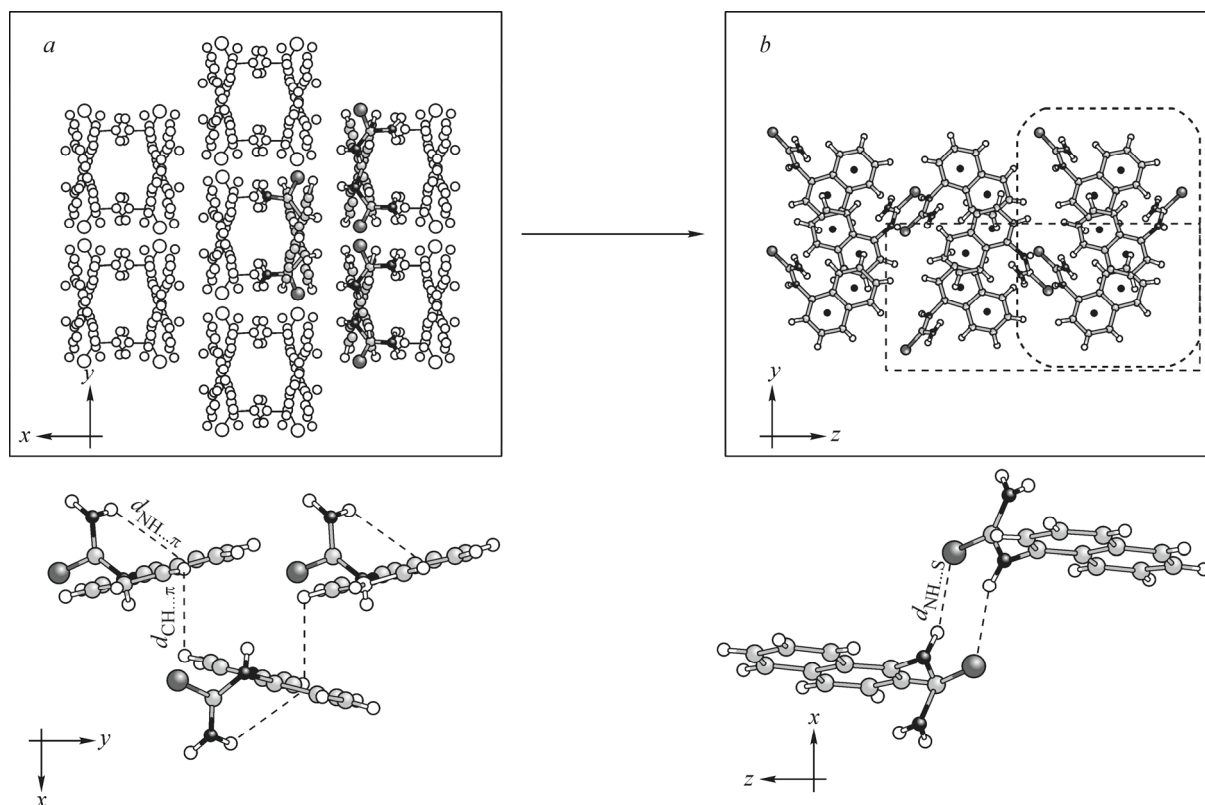


Fig. 2. The first figured approach to analyze the interactions in the lattice. The lattice system with selected moieties (colored) to study their interaction inside the complete lattice represented without color (a), clear view on the yz plane for the moieties in (a), (below) view on the xy plane for the interactions circled as dotted cyclic-box in (b), and view on the xz plane for the intramolecular hydrogen bonding found in the dashed box in (b)

Calculation results. Geometric parameters of the optimized structures of **1** at the B3LYP/*cc-pVTZ*, RHF/*cc-pVTZ*, RIMP2/*cc-pVDZ* and RIMP2/*cc-pVTZ* levels are listed in Table 3. As shown in Table 3, the calculated bond distances and angles agree well with those in the crystallographic data. The largest deviations between the theoretical and X-ray geometries are mainly in the thiourea unit. In the naphthalene rings, the largest deviation of the bond distances reaches 0.02 Å (all methods, C—H bond lengths). The hydrogen atoms in X-ray geometries are located using the riding model. This model has a larger error in locating hydrogen atoms than *ab initio* methods. In addition, the calculations at the B3LYP/*cc-pVTZ* and RIMP2/*cc-pVTZ* levels could almost predict the intermolecular geometry in **1**. In the case of HF, a large deviation in torsion angles was found to take place. The C1—N2—C10—C11 and C1—N2—C10—C9 torsion angles are 77.08° and 106.24° respectively in X-ray geometries, 92.23° and 88.95° using RHF/*cc-pVTZ*, 75.65° and 106.4° using B3LYP/*cc-pVTZ*, and 70.72° and 110.8° using RIMP2/*cc-pVTZ*. Another important feature in the calculations is the aminic bonds. The H—N—H...C10 distance is 2.429 Å and almost equal to that at the RIMP2/*cc-pVTZ* level of calculations (2.414 Å). In general, the thiourea tail is best produced at B3LYP and RIMP2 levels of theory than that with HF. The energies calculated at the RHF, B3LYP, and MP2 levels are -929.0 kJ/mol, -933.1 kJ/mol, and -931.3 kJ/mol respectively. Finally, the Mulliken population analysis at RIMP2/*cc-pVTZ* shows that the charge is mainly on the nitrogen atoms and sulfur as expected.

The next step is to calculate the S...H—N interaction energies. In the literature, RIMP2 is the model of choice [20] and so we use it here for the same purpose. Although the riding model in SHELXTL fixes hydrogen atoms, we use the X-ray data as a starting model to obtain the intermolecular interaction energy of S...H—N to best estimate the energy at this distance. The molecular dimer of

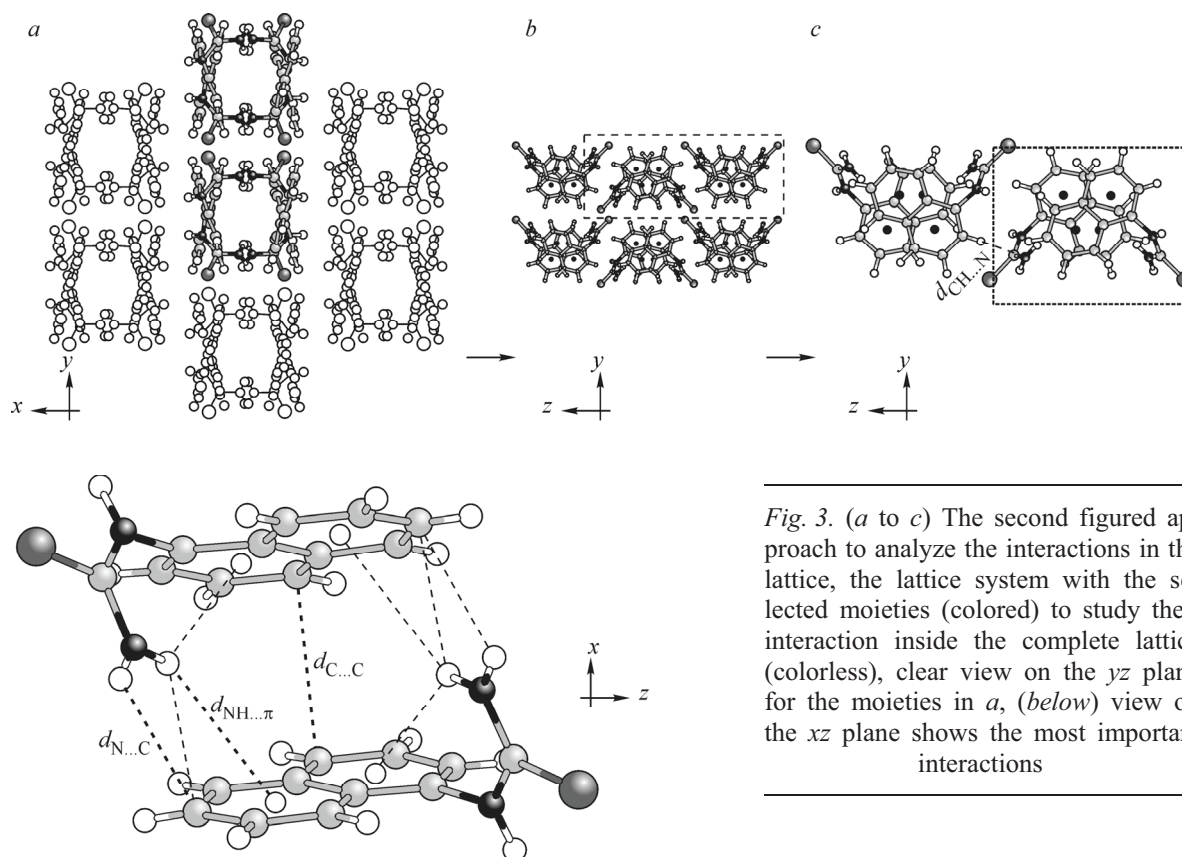


Fig. 3. (a to c) The second figured approach to analyze the interactions in the lattice, the lattice system with the selected moieties (colored) to study their interaction inside the complete lattice (colorless), clear view on the yz plane for the moieties in a, (below) view on the xz plane shows the most important interactions

two molecules of **1** (Fig. 3(below)) has interaction energies of -36.1 kJ/mol and -41.7 kJ/mol reproduced at the X-ray//RIMP2/ cc - p VDZ and cc - p VTZ levels of theory respectively, and including the BSSE correction. The value is in the range of strong S...H—A hydrogen bonding interactions and up to our knowledge it is the strongest reported in the literature, comparable to the energy in AH...SO₂ interactions [21, 22]. Also, the obtained value is in the range of H₂S...HF (-30.24 kJ/mol, MP2/6-311++G(d,p)) [8]. Other examples of S...H—O systems can be found in [23]. The other calculated N—H...S interaction energies in other systems reported in the literature are few. For example, N—H...S hydrogen-bonded complexes of the model compounds of tryptophan (indole and 3-methylindole) among other derivatives have been calculated [24]. Their values are in the range of the values reported in this article.

CONCLUSIONS

We analyzed the crystal structure of 1-(1-naphthyl)-2-thiourea. This molecule is well known in the literature, however up to our knowledge this is the first time that its crystal structure is solved. The crystal structure reveals an interesting hydrogen bonding of sulfur with an S...N distance of 3.196 Å. This type of noncovalent bonding is worth of studying since thiol is involved in many biological molecules and energy data is important to be known. We analyzed the unimolecular system and three levels of calculations were used for this purpose. RHF, B3LYP, and RIMP2 were found to be the best in producing the X-ray geometry. The interaction energy was collected at the RIMP2 level of theory using two basis sets. These energies were -36.1 kJ/mol and -41.7 kJ/mol with cc - p VDZ and cc - p VTZ basis sets respectively and including the BSSE correction. This value shows that the S...H—N noncovalent interaction in this system is one of the strongest found in the literature.

Supplementary material. Full distances and angles obtained from X-ray, HF, B3LYP and RIMP2, along with Mulliken analyses at different levels have been supplemented.

CCDC contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html> (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033).

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