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RESEARCH ARTICLE

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Synthesis, crystal structure, hydrogen bonding interactions analysis of novel acyl thiourea derivative

Xing Zhang¹ | Xiaoli Du² | Jirong Song³ | Jie Huang¹

¹School of Chemical Engineering, Northwest University/Shaanxi key Laboratory of Physico-Inorganic Chemistry, Xi'an, Shaanxi, China
²Yuyang District Food Inspection and Testing Center, Yulin, Shaanxi, China

³Ministry of Science and Technology, The Palace Museum, Beijing, China

Correspondence

J. Huang, School of Chemical Engineering, Northwest University/Shaanxi Key Laboratory of Physico-Inorganic Chemistry, Xi'an, Shaanxi 710069, China. Email: huangjie@nwu.edu.cn

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Abstract

The N-(p-methoxybenzoyl)-N'-(2,4-dinitrophenyl amino)thiourea has been synthesized and characterized by FT-IR, ¹H NMR, and elemental analyses techniques. Also, its molecular structure was determined by single-crystal Xray diffraction. It revealed that the title compound crystallizes with two unique molecules in the asymmetric unit of the orthorhombic unit cell, space group Pna2(1) with a = 18.857(5) Å, b = 8.148(2) Å, c = 22.443(6) Å, $\beta = 90.00^{\circ}$, $C_{15}H_{13}N_5O_6S$, $M_r = 391.36$, V = 3448.2(15) Å³, Z = 8, $D_c = 1.508$ g·cm⁻¹, $F(000) = 1616, \mu = 0.233 \text{ mm}^{-1}, S = 1.06$, the final R = 0.0626, and wR (I > 2(I))= 0.1392. Intramolecular N-H ... N, C-H ... N, and N-H ... O hydrogen bonds indicate that the molecule conformation was mostly planar. Crystal structure stacking through the N-H ... O, C-H ... O, and N-H ... S hydrogen bonds, and two π ... π interactions arrangement revealed their conspicuous role in the stabilization of the molecular structure. The type and nature of intermolecular interactions in the crystal structure were investigated by Hirshfeld surfaces and their associated two-dimensional fingerprint plots. Furthermore, shape index and curvedness surfaces further confirmed $\pi \dots \pi$ stacking interactions with different features of molecule A and B. More importantly, the reduced density gradient (RDG) function provides a real-space function for discussing noncovalent interactions (NCI) in title compound, including van der Waals interactions and C–H ... π contacts in addition to hydrogen bonding interactions within molecule.

KEYWORDS

crystal structure, Hirshfeld surface analysis, noncovalent interactions, novel thiourea derivative

1 | INTRODUCTION

Thiourea has interesting behavior due to its unique combination of functional group, including amino, imino, and thiol.^[1] Acyl thiourea is a class of important derivatives of thiourea. On the other hand, acyl thiourea derivatives are widely applied in recent decades, such as heterocyclic synthesis intermediate, non-ionic surfactants, organocatalysts, etc. Further, due to the unique structure of —CO—NH—CS—NH— in the structure of the acyl thiourea compound, it has a wide range of biological activities, such as antiviral,^[2–4] antimicrobial,^[5–7] herbicidal,^[8] antitumor,^[9] anti-inflammatory,^[10,11] and fungicidal properties.^[12] However, an increasing number of people are engaged in researching anticancer drugs as cancer cases have become more diverse and complex. Thus, acyl thiourea derivative was also used to study pharmacological activity through molecular docking methods by our research group.^[3] Very recently, supramolecular chemistry has developed rapidly, so the research of acyl thiourea began to identify supramolecular anions, and the development of self-assembled materials has become the focus of the scientific community.^[13] In addition, thiourea derivatives are exceptionally versatile ligands in coordination chemistry, due to the existence of O, S, and N donor atoms in the central thiourea group moiety; it often facilitates to form complexes with various transition metals.^[14–17]

The 3D-Hirshfeld surface analysis^[18] and 2D fingerprint plots^[19] are becoming effective tools for discussing intermolecular hydrogen bonding interactions and maintaining self-assembly of supramolecules.^[20] According to recent related literature reports, Hirshfeld surfaces analysis explains and evaluates intermolecular hydrogen bonding interactions in a series of thiourea derivatives.^[21,22] Besides, the type and intensity of noncovalent interaction (NCI) can be visually analyzed by electron density and reduced density gradient (RDG) function.^[23,24] Apart from the hydrogen bonding interactions, the NCI analysis reveals the presence of other weak NCIs such as C–H ... π lone pair, C–H ... π contacts, Van der Waals interactions, and steric hindrance in the solid state structure of acyl thiourea derivatives.^[25,26] Thence, the NCIs in the crystal of compound play an important role in stabilizing molecules with a special mode of action, and it is worthwhile to our attention.^[27]

Based on the above facts, we intend to report the preparation, characterization, and crystal structure of *N*-(pmethoxybenzoyl)-*N*'-(2,4-dinitrophenyl amino)thiourea. Molecular and structural characterization were carried out by FT-IR, ¹H NMR, and X-ray crystallographic studies. In order to precisely quantify those intermolecular contacts and analyze packing features, we also use the Hirshfeld surface analysis, 2D fingerprint plots, shape index, and curvedness properties. Moreover, the NCIs were investigated by electron density and RDGs.

2 | EXPERIMENTAL

2.1 | Measurements and instruments

All reagents and solvents for synthesis and analysis were commercially available obtained from Sigma Aldrich. Reagents were purified according to the standardization process and used without further purification. Microwave synthesis was carried out using a BILON-CW-1000 microwave synthesizer with the appropriate absorption power setting. The melting point was determined on a Cossim KER3100-08S apparatus. The FT-IR (KBr pellets) spectrum was recorded in the 4000 to 400 cm⁻¹ range using a Bruker EQUINOX 55 FT-IR spectrometer. The ¹H nuclear magnetic resonance (NMR) spectrum of the title compound was determined in dimethylsulfoxide-d₆ at 400 MHz using a Bruker spectrophotometer. Elemental analyses were performed employing an ELEMENTAR Vario EL III elemental analyzer.

2.2 | Synthesis of *N*-(p-methoxybenzoyl)-*N*'-(2,4-dinitrophenyl amino) thiourea

A solution of prepared 4-methoxybenzoyl chloride (1.7059 g, 10 mmol) in dry tetrahydrofuran (40 mL) was added dropwise to a three-necked round-bottomed flask containing potassium thiocyanate (1.4577 g, 15 mmol). The reaction mixture was refluxed for approximately 2 hours at 60°C. A solution of 2,4-dinitrophenylhydrazine (2.2329 mL, 9.5 mmol) in tetrahydrofuran (20 mL) was added and reacted in microwave heating 60°C to 65°C for about 3 minutes. After the reaction was completed, the resulting mixture in the flask was poured into a beaker containing 600 mL of cold water and filtered off, washed with ethanol, and dried in vacuo. A suitable crystal of the title compound for crystal structure determination was obtained upon slow evaporation at room temperature from 15 mL of an organic solvent (ethanol and ethyl acetate = 2: 1) after a week. The synthesis route of the compound was performed according to Scheme 1.

The title compound was obtained as white block crystal. Yield: 2.86 g, 87%; m.p.: 189.4°C to 190.7°C; anal. calcd for $C_{15}H_{13}N_5O_6S$ ($M_r = 391.36$): C, 46.03; H, 3.35; N, 17.89%. Found: C, 46.52; H, 3.48; N, 17.27%. FT-IR (KBr): ν , cm⁻¹ 3396/3262 (m, N—H stretching), 2979 (m, C—H stretching), 1676 (s, C=O stretching), 760 (s, C=S stretching). ¹H NMR (400 MHz, DMSO-d₆): δ 11.68 (s, 1H, NH), 10.56 (s, 1H, NH), 8.89 (s, 1H, Ar—H), 8.36 (s, 1H, Ar—H), 8.03 (s, 2H, Ar—H), 7.29 (s, 1H, Ar—H), 7.02 (s, 2H, Ar—H), 3.87 (s, 3H, OCH₃).



SCHEME 1 Synthetic route for the synthesis of the target compound

2.3 | Crystal structure analysis

A white block crystal with dimensions of 0.37 mm × 0.25 mm × 0.13 mm was chosen for X-ray determination analysis. Single crystal X-ray experiment was carried out by Mo $K\alpha$ radiation ($\lambda = 0.071073$ nm) with Bruker APEX-II CCD diffractometer.^[28] Molecular structure was generated by the MERCURY program.^[29] SHELXS 97 was used for structure solution and refinement by full-matrix least squares on F^2 using the direct methods.^[30] Moreover, the structural stacking diagram of the compound was displayed using a Diamond software program, and additional geometrical calculations were calculated using the program PLATON program.^[31]

2.4 | Computational details

The plots of the RDG versus the electron density multiplied by the sign of the second Hessian eigenvalue sign (λ_2) were presented by Multiwfn and VMD 1.9.1 software.^[32,33] The NCI map is based on a visual index of electron density and its derivatives, which can effectively identify and visualize NCI regions in molecular structures. Consequently, the peaks that appear in the RDG at low densities correspond to the different NCIs in 2D plots.

3 | RESULTS AND DISCUSSION

3.1 | Spectroscopic data

The infrared spectra of the title compound showed that the absorptions of N—H groups were located at 3262 to 3396 cm⁻¹ regions. At the same time, the stretching vibration of C=S is assigned at 760 cm⁻¹. The stretching vibration C=O occurred to strongest absorption peaks at 1676 cm⁻¹ and a strong 1320, 1243 cm⁻¹ absorption peak, which is attributed to the stretching vibration of C–N single bonds in the title compound. In the ¹H NMR spectrum of the ligand shows singlet peaks for phenyl NH proton at 11.68 ppm and the amide NH proton at 10.56 ppm, respectively. However, the nitro group is a strong electron-withdrawing group, which can reduce the electron density of nearby hydrogen nuclei and increase the hydrogen displacement on the benzene ring. Thus, the H2 atom was observed as a single peak at 8.89 ppm. The protons of benzene rings are observed at 7.05 to 8.03 ppm and the proton of methoxy group appeared at 3.87 ppm in the title compound. Surprisingly, H4C atom may be too active to observe in the hydrogen spectrum of the acyl thiourea derivative.

3.2 | Crystal structure analysis

The title compound crystallized in the orthorhombic system with two discrete molecules, A and B, in the asymmetric unit cell, as is shown in Figure 1. Crystal data, data collection, and structure refinement details are summarized in Table 1. The selected crystal bond lengths and bond angle geometric parameters were in the allowed ranges, as given in Table 2. Interestingly, the properties of the two molecules are highly similar. However, there are slight differences between the two molecules mainly in the partial bond lengths, bond angles and the dihedral angles of the plane where the respective benzene ring and pyrimidine ring located. The bond lengths of C(7)-N(5) and C(22)-N(10) of the title compound are 1.385(5) and 1.405(6) Å, respectively. At the same time, the nitro group [O(3)-N(2)-O(4)] in structure A has poor planarity with the benzene ring [C(1)-C(6)], whereas the corresponding O(7)—N(6)—O(8) in structure **B** is close to coplanar with the benzene ring [C(16)-C(21)], with dihedral angles between the benzene ring planes and the nitro meanplanes of 12.967° for molecule A and 4.303° for molecule **B**. Besides, the bond lengths of N(4)—C(7), C(7)—N(5), and N(5)-C(8) are 1.333(6), 1.385(5), and 1.383(6) Å, which illustrated a conjugation among the N(3), N(4), C(7), N(5),



FIGURE 1 Molecular structure of the title compound

TABLE 1 Crystal data and structure refinement parameters statistic for compound

CCDC	1439535
Chemical formula	$C_{15}H_{13}N_5O_6S$
Formula weight	391.36
Temperature (K)	296(2)
Wavelength (Å)	0.71073
a (Å)	18.857(5)
b (Å)	8.148(2)
<i>c</i> (Å)	22.443(6)
α (degree)	90
β (degree)	90
γ (degree)	90
Volume (Å ³)	3448.2(15)
Z	8
Dc (Mg/m ³)	1.508
Crystal system	Orthorhombic
Space group	Pna2(1)
Index ranges	$-18 \le h \le 22, -8 \le k \le 9, -26 \le l \le 26$
Absorption coefficient (μ)	0.233
F(000)	1616
The range for data collection (°)	1.81 to 25.10
Reflections collected	6116
Independent reflections	3993
R _{int}	0.075
Goodness-of-fit on $F^2(S)$	1.062
R (all data)	$R_1 = 0.0626, wR_2 = 0.1392$

$\label{eq:constraint} \textbf{TABLE 2} \quad \ \ \text{Selected bond lengths} (\text{\r{A}}) \ \text{and bond angles} (^{o})$

Bond	Dist.	Bond	Dist.	Bond	Dist.
S(1)—C(7)	1.655(5)	C(7)—N(5)	1.385(5)	C(22)—N(9)	1.339(6)
N(3)—N(4)	1.385(5)	C(8)—N(5)	1.383(6)	C(23)—O(11)	1.214(6)
C(7)—N(4)	1.333(6)	S(2)—C(22)	1.645(5)	C(22)—N(10)	1.405(6)
C(6)—N(3)	1.346(6)	N(8)—N(9)	1.393(5)	C(23)—N(10)	1.382(7)
C(8)—O(5)	1.235(6)	C(21)—N(8)	1.352(6)		
Angle	(°)	Angle	(°)	Angle	(°)
C(8)-N(5)-C(7)	128.9(4)	O(5)-C(8)-C(9)	121.9(5)	C(21)—N(8)—N(9)	120.0(4)
N(4)-C(7)-S(1)	123.8(4)	C(5)—C(6)—N(3)	119.9(4)	N(10)-C(23)-O(11)	122.2(5)
C(6)—N(3)—N(4)	121.3(4)	C(23)—N(10)—C(22)	127.3(5)	O(11)-C(23)-C(24)	121.2(5)
N(5)-C(8)-O(5)	120.8(5)	N(9)—C(22)—S(2)	124.6(4)	C(20)-C(21)-N(8)	123.2(5)

and C(8) atoms. Meanwhile, the N(8)–N(9), N(9)–C(22), C(22)–N(10), and N(10)–C(23) bond lengths (see Table 1) indicate that the N(8), N(9), C(22), N(10), and C(23) atoms

have conjugate relations. Therefore, the compounds are sufficiently similar for their molecular structures to be discussed together. Intramolecular and intermolecular hydrogen bond parameters are listed in Table 3. It is not difficult to find that the compound possesses intramolecular N(3)—H (3)…O(1), N(4)—H(4C)…O(5), N(9)—H(9)…O(11), and N(8)—H(8)…O(10) hydrogen bonds that form sixmembered rings and contribute to the relative planarity of the thiourea central part skeleton. Moreover, an intramolecular hydrogen bond has been observed between C and N atoms [C(5)—H(5)…N(4), C(16)—H(16)…N(9)], as

TABLE 3 Hydrogen-bond geometry for the title compound (Å and $^{\circ}$)

D—H…A	d (D—H)	d (H…A)	d (D…A)	∠ (D—H…A)
N(3)—H(3)…O(1)	0.86	1.97	2.591(6)	128
N(3)—H(3)…N(1)	0.86	2.61	2.916(7)	103
N(4)-H(4C)···O(5)	0.86	1.92	2.598(5)	134
N(8)—H(8)…N(7)	0.86	2.61	2.904(7)	102
N(8)-H(8)O(10)	0.86	1.97	2.596(6)	128
N(9)−H(9)…O(11)	0.86	1.91	2.585(6)	134
C(5)-H(5)···N(4)	0.93	2.46	2.783(7)	100
C(16)-H(16)N(9)	0.93	2.40	2.737(7)	101
N(10)—H(10C)…O(1) ^a	0.86	2.43	3.258(6)	161
$C(11) - H(11) - O(11)^{b}$	0.93	2.48	3.369(7)	159
$C(14) - H(14) - O(10)^{c}$	0.93	2.55	3.442(7)	160
C(15)-H(15B)····O(3) ^d	0.96	2.46	3.273(7)	142
$C(16) - H(16) - O(4)^{e}$	0.93	2.59	3.237(8)	127
$C(25) - H(25) - O(1)^{a}$	0.93	2.53	3.437(7)	164
$C(28) - H(28) - O(5)^{e}$	0.93	2.51	3.405(6)	160
N(3)-H(3)···S(2) ^f	0.86	2.66	3.299(4)	132
C(4)-H(4)···O(7) ^g	0.93	2.58	3.202(7)	125
N(5)-H(5C)···O(10) ^c	0.86	2.51	3.330(6)	159
N(8)-H(8)···S(1) ^h	0.86	2.68	3.298(5)	129

shown in Figure 1. The packing diagram of the synthesized compound is depicted in Figure 2. The crystal structure of the title compound has a pair of N-H...S hydrogen bonds, corresponding to the N(8)-H(8)...S (1) (x, -1 + y, 1 + z) and N(3)-H(3)...S(2) (x, y, -1 + z)intermolecular hydrogen bond forming R2 2(10) closed ring motif (expressed with a red dotted line). Two molecules in the asymmetric unit are also stabilized by N(5) - H(5C) - O(10) (x, y, 1 + z) and N(8) - H(8) - S(1)generating with an R2 2(10) closed ring motif (expressed with a blue dotted line). In addition, O(10) atom acts as a receptor and is connected to form R1 2(7) ring motif (expressed with a pink dotted line) by two types of intermolecular hydrogen bonds C(14)-H(14)...O(10) (x, y, 1 + z)and N(5)-H(5C)-O(10), respectively. They further encapsulate in the case larger R2 2(10) ring motif (expressed with a green dotted line) via the N(10)-H $(10C)\cdots O(1)(x, y, -1 + z)$ and N(3)-H(3)···S(2) hydrogen bonds linking adjacent A and B molecules. Apart from this series of intermolecular contacts, the two molecules were also stabilized through $\pi \cdots \pi$ stacking contacts, respectively, as shown in Figure S1. The center Cg(1)—Cg (2) [Cg(1):C(1)-C(6), Cg(2):C(9)-C(14)] distance is 3.682° in the molecule structure **A**. Similarly, the benzene ring in structure \mathbf{B} is interlaced with the benzene ring in the compound of the adjacent layer, and the center $Cg(3)^{\circ}Cg(4)$ [Cg(3):C(16)^{\circ}C(21), Cg(4):C(24)^{\circ}C(29)] distance is 3.698° that corresponds to forming a face-toface $\pi \cdots \pi$ stacking interactions (see Figure S1). Therefore, abundant hydrogen bonding could be formed in the crystal structure, and the presence of these intramolecular and intermolecular hydrogen bonds made the title compound more stable.

Symmetry codes: (a) x, 1 + y, -1 + z; (b) 2 - x, 1 - y, 0.5 + z; (c) x, y, 1 + z; (d) 1 + x, y, z; (e) 1.5 - x, 0.5 + y, -0.5 + z; (f) x, -1 + y, 1 + z; (g) 2 - x, 2 - y, 0.5 + z; (h) x, y, -1 + z



FIGURE 2 Packing diagrams of the title compound viewed along the *b*-axis

3.3 | Hirshfeld surface analysis

In order to understand the title compound interactions within the crystal structure, the Hirshfeld surface analysis and their associated 2D fingerprint plot were performed using CrystalExplorer 3.1 program software.^[34-36]

The Hirshfeld surfaces mapped over the d_{norm} were seen in Figure 3. From the view of d_{norm} surfaces for the title compound, some red areas could be observed. The $d_{\rm norm}$ map shows red regions labeled 1 for molecule A, labeled 6 for molecule **B**, which demonstrate strong N-H...S [N(8)-H(8)...S(1) and N(3)-H(3)...S(2)] intermolecular hydrogen bonding interactions. The two red regions labeled 2 and 5 in the d_{norm} map are attributed to N-H...O contacts, which is N(5)-H(5C)...O(10) and N(10)-H(10C)...O(1) hydrogen bonding interactions. Similarly, we observe red regions appear near to the carbon atom (labeled 3 and 4), which correspond to intermolecular C(11)-H(11)...O(10) and C(25)-H(25)...O(1) hydrogen bond interactions. For molecule A, the lightest red region (labeled 7) is attributed to the C(4)-H(4)...O (7) contacts. The C···O contacts attributed to C(14)-H $(14)\cdots O(10)$ and C(15)-H $(15B)\cdots O(3)$ hydrogen bonds can be seen as the two red regions labeled 8 and 9. Meanwhile, the red regions occur near to the O and C atoms in the compound **B**, respectively, which are due to form C(11)- $H(11)\cdots O(11)$ and $C(28)-H(28)\cdots O(5)$ intermolecular hydrogen bonding interactions (labeled 10 and 11) with adjacent molecules.

Fingerprint plots in Figure S2 revealed the intermolecular interaction patterns and the relative contributions to the Hirshfeld surface of the synthesized compound. The upper spike (labeled 1) corresponds to the donor spike, while the lower spike (labeled 2) corresponds to an acceptor spike, as illustrated in Figure S2 (a). The S…H/H…S (10.5%) contacts with a pair of sharper spikes center near to a sum of $(d_i + d_e)$ 2.5 Å are presented in Figure S2, which are attributed to the N(8)-H(8)...S(1) and N(3)-H(3)...S(2) hydrogen bond interactions. The O···H/H···O (3.7%) contacts with a pair of sharp spikes center near to a sum of $(d_i + d_e)$ values were about 2.3 and 2.5 Å in the fingerprint plots. Interestingly, the O···H/H···O contacts contributed the most to the entire Hirshfeld surfaces of the title compound. The conventional H...H contacts contribute 18.4% on the Hirshfeld surface with a pair of sharp spikes between $(d_i + d_e)$ 2.1 and 2.3 Å. However, Figure S2 depicted that C…C contacts (4.9%) appear at spikes center near to a sum of $(d_i + d_e)$ 2.4 and 2.5 Å, which is due to the $\pi \cdots \pi$ stacking interactions in the molecules. Besides, the N…H/H…N (1.5%) and C…H/H…C (10.0%) intermolecular contacts also contribute to the Hirshfeld surfaces, as shown in Table S1.

The shape index and curvedness properties generally used to identify planar stacking arrangements were performed in the compound A and B, respectively, as shown in Figure 4. For molecular structure A, the red-blue triangles were presented in phenyl regions [C(1)-C(6)] of shape index, which indicated that the entire surface is $\pi \cdots \pi$ stacking interactions with adjacent molecular. At the same time, the red-blue triangle appears in the benzene ring [C(16)-C(21)] region of the compound structure **B**, which is due to the presence of $\pi \cdots \pi$ stacking interactions between the adjacent two molecules (seen in Figure S1). It can be observed in Figure 4, the flat regions of the curvedness surface also indicate the $\pi \cdots \pi$ stacking interactions. Therefore, apart from these nonclassic hydrogen bonds, C...C contacts atoms of the molecule inside the surface of the synthesized compound A and **B** also attribute to the $\pi \cdots \pi$ stacking interactions, as shown in Figure S2 (g).



FIGURE 3 Hirshfeld surfaces d_{norm} for molecules A and B



FIGURE 4 The shape index (the left) and curvedness (the right) for molecules A and B

3.4 | Noncovalent interaction analysis

The NCI theory identifies interactions as areas of low electron density (ρ) and low RDGs. The RDG function is usually used to better understand and highlight the regions involved in the weak interaction in the whole molecular system, so as to intuitively analyze which regions are related to the weak interactions. This weak interaction was distinguished by the values of sign (λ_2) ρ and color coded, whereas the sign (λ_2) ρ function is the symbol of the second largest eigenvalue λ_2 of the electron density Hessian matrix. Blue isosurfaces show the strong attractive interaction such as hydrogen bond and strong halogen bond. Conversely, green areas indicate the weak regions exhibit strong mutual exclusion interactions.

The NCI analysis has been performed to identify interactions in hydrogen bonded compound, while this weak interaction of the title compound is generated and represented by the 2D NCI map and the 3D isosurface. The 3D isosurface plot was given in Figure 5, and the spikes of 2D NCI plot of the reduced gradient values sign $(\lambda_2)\rho$ were shown in Figure 6. For the title compound, red fusiform shapes were observed in the central regions of the two benzene rings, respectively (Figure 5). It reflected strong steric effect between the benzene rings, corresponding to a clear peak on the scatter plot (Figure 6). There is a blue isosurface between the nitrogen atom and the oxygen atom. It belongs to the N-H…O strong hydrogen bonding interaction, which corresponds to -0.040 a.u. < sign $(\lambda_2)\rho < -0.032$ a.u. in the 2D NCI plot. The N-H--N and C-H--N hydrogen bond contacts displayed the low gradient low density interaction with values of -0.040 a.u. < sign (λ_2) ρ < -0.030 a.u. and -0.020 a.u. < sign (λ_2) $\rho < -0.015$ a.u., respectively, as shown in Figure 6. There is a low density domain coming from C-H--O=C attractive interactions in the range of -0.040 a.u. to -0.030 a.u.. This is in good agreement with the previously reported results.^[25] In particular, an area of flat bicolored proved that attractive and exclusive interactions synchronously existed between S and H atoms, as shown in Figure 5. It was worth noting that the weak vdW interactions appeared at the position where -0.005 a.u. < sign (λ_2) $\rho < 0.005$ a.u., as shown in



FIGURE 5 The title compound 3D gradient isosurface structure



FIGURE 6 The title compound 2D NCI plots

Figure 6. Similarly, the NCI analysis revealed the presence of another C—H—N interactions with 0.010 a.u. < sign (λ_2) ρ < 0.015 a.u. in the 2D NCI plot. Herein, the attractive can be attributed to C—H—lone pairs interactions owing to unpaired electrons on the N atoms. The weak C—H—O interactions exist between C and O atoms, with values of -0.020 a.u. < sign (λ_2) ρ < -0.010 a.u. Besides, the other RDG isosurfaces with flat bicolored characteristics of the title compound also express various attractive and repulsive effects.

4 | CONCLUSION

N-(p-methoxybenzoyl)-N'-Novel title compound (2, 4-dinitrophenyl amino) thiourea has been synthesized and characterized. The structural and conformational properties of the title compound were determined by Xray single crystal diffraction. These intramolecular and intermolecular interactions have certain profound significance in stabilizing the molecular structure. The Hirshfeld surfaces and 2D fingerprint plots were carried out to clearly confirm the intermolecular interactions and their quantitative contributions to the crystal packing of the title compound. The presence of significant NCIs of the molecule system was clarified based on detailed RDG function and NCI analysis. These intramolecular and intermolecular interactions have certain profound significance in stabilizing the molecular structure.

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ORCID

Jie Huang D https://orcid.org/0000-0003-3561-2819

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

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