

Crystal structure, Hirshfeld surface analysis and DFT studies of 2-[4-(2-methylpropyl)phenyl]-*N'*-(1*Z*)-1-(thiophen-2-yl)ethylidene]propanehydrazide

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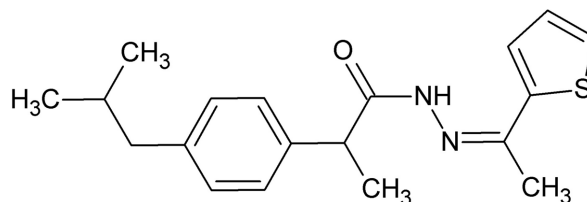
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In the title compound $C_{19}H_{24}N_2OS$, intermolecular $N-H\cdots O$ hydrogen bonds generate $R_2^2(8)$ ring motifs, forming dimers with an interaction energy of -70.5 kJ mol^{-1} . A short $S\cdots C$ interaction produces another dimer with an interaction energy of -30.6 kJ mol^{-1} . The intermolecular interactions were quantified using Hirshfeld surface analysis. The two-dimensional fingerprint plots indicate that the major contributions to the crystal packing are from $H\cdots H$ (67.9%), $C\cdots H$ (13.7%), $O\cdots H$ (7.3%) and $S\cdots H$ (4.3%) interactions.

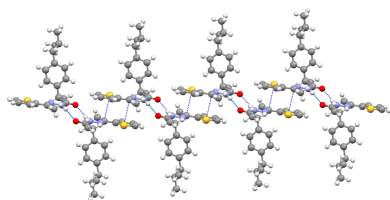
1. Chemical context

Derivatives of ibuprofen have been synthesized to enhance the efficacy and reduce the side effects commonly associated with traditional NSAIDs (Ahmadi *et al.*, 2017). These derivatives have shown promising results in preliminary studies, particularly regarding anti-inflammatory, analgesic, and antimicrobial activities (Sujith *et al.*, 2009; Dhakane *et al.*, 2014). Compared to other derivatives of NSAIDs, ibuprofen hydrazides may offer distinct advantages, although comprehensive clinical comparisons are still limited (Kamms & Hadi, 2023). Based on the above studies, we herein report the crystal structure of the ibuprofen hydrazide derivative 2-[4-(2-methylpropyl)phenyl]-*N'*-(1*Z*)-1-(thiophen-2-yl)ethylidene]propanehydrazide (**1**).



2. Structural commentary

The title compound crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the asymmetric unit (Fig. 1). The lengths of the $C-S$ bonds $C16-S1$ and $C19-S1$ are 1.7225 (14) and 1.7115 (18) Å, respectively, while the carbonyl bond distance $C13-O1$ is 1.2297 (15) Å. The torsion angle $N1-N2-C14-C16$ is $176.95(10)^\circ$, while $C8-C11-C13-O1$ is $103.88(14)^\circ$. The benzene (*A*, $C5-C10$; r.m.s.d. = 0.004 Å) and thiophene (*B*, $C16-C19/S1$; r.m.s.d. = 0.004 Å) rings are not coplanar, subtending a dihedral angle of $86.69(4)^\circ$.



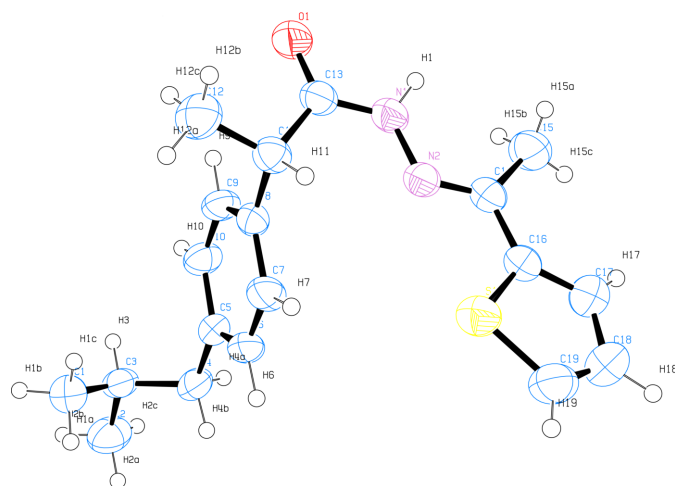


Figure 1
The molecular structure of **1** with displacement ellipsoids drawn at the 50% probability level.

3. Supramolecular features

In the crystal, N1—H1...O1 hydrogen bonds [2.119 (18) Å; Table 1] lead to the formation of dimers with an $R_2^2(8)$ motif. Energy calculations at the B3LYP/6-31G(d, p) level were performed using *Crystal Explorer 21.5* (Mackenzie *et al.*, 2017; Spackman *et al.*, 2021) software with the CIF as the input file. The dimer energy was found to be $-70.5 \text{ kJ mol}^{-1}$. In the crystal, each molecule in the dimer also forms an S1...C14 short interaction [3.5214 (14) Å; symmetry operation $-x, 2 - y, 2 - z$], forming another dimer with an $R_2^2(6)$ motif and thereby forming a chain running in the b -axis direction (Fig. 2). The energy of the dimer formed by this short interaction was calculated to be $-30.6 \text{ kJ mol}^{-1}$.

4. Hirshfeld surface analysis

Hirshfeld surface analysis (Hirshfeld, 1977; Spackman & Jayatilaka, 2009) was conducted using *Crystal Explorer* (Spackman *et al.*, 2021) to visualize and quantify the intermolecular interactions in the title molecule. The Hirshfeld

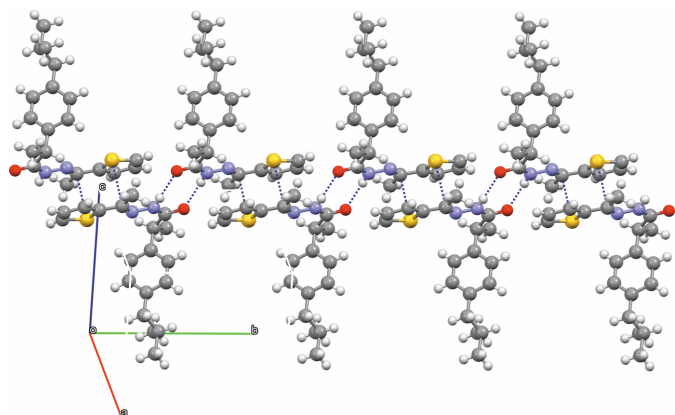


Figure 2
A chain of molecules in the crystal structure of **1**.

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1...O1 ⁱ	0.859 (18)	2.119 (18)	2.9537 (15)	163.6 (16)

Symmetry code: (i) $-x, -y + 3, -z + 2$.

surface for the title compound mapped over d_{norm} is shown in Fig. 3. The red region is attributed to the N1—H1...O1 interaction. The two-dimensional fingerprint plots in Fig. 4

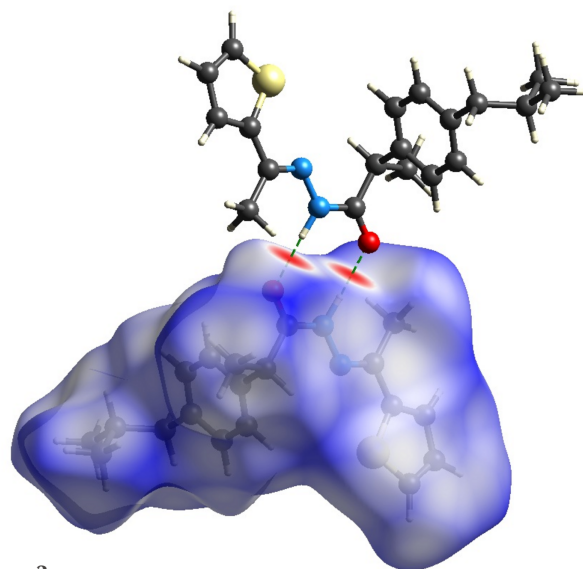


Figure 3
The Hirshfeld surface of the title compound mapped over d_{norm} with dashed lines indicating the N—H...O hydrogen bonds that lead to the formation of dimers.

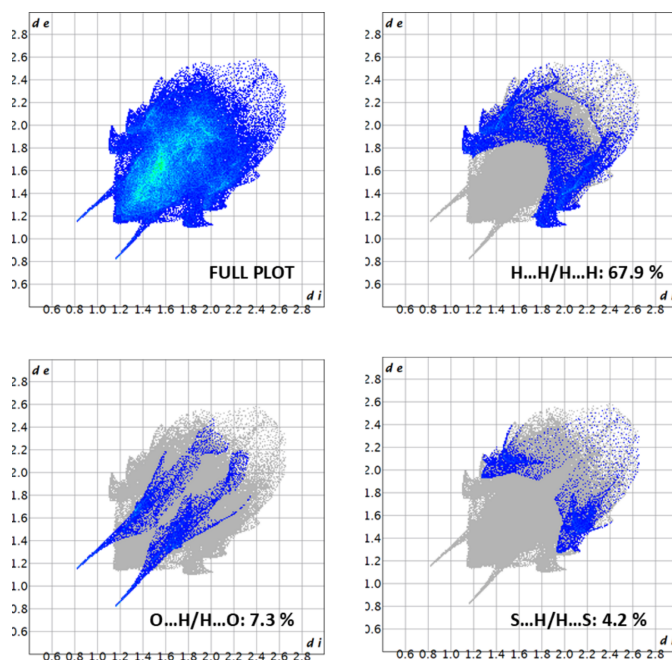


Figure 4
The two-dimensional fingerprint plots of the title molecule, showing all interactions and those delineated into H...H, O...H/H...O and S...H/H...S.

indicate that the major contributions to the crystal packing are from H $\cdots$ H (67.9%), C $\cdots$ H (13.7%), O $\cdots$ H (7.3%) and S $\cdots$ H (4.3%) interactions.

5. Database Survey

A search of the Cambridge Structural Database (CSD, updated to January 2025; Groom *et al.*, 2016) for the 2-(4-isobutylphenyl)-*N'*-methylpropanehydrazide moiety yielded two closely related structures: 1-[2-(4-isobutylphenyl)propanoyl]thiosemicarbazide (**2**; CSD refcode HOLQIJ; Fun & Kia *et al.*, 2009) and *N*-(2,4-dioxo-1,3-thiazolidin-3-yl)-2-(4-isobutylphenyl)propanamide (**3**; CSD refcode HUCTUV; Fun & Goh *et al.*, 2009). In compound **2**, the crystal structure features N—H $\cdots$ O and N—H $\cdots$ S hydrogen bonds, with donor–acceptor distances of 2.09 (15) and 2.495 (13) Å, respectively, leading to a supramolecular architecture. In compound **3**, the supramolecular structure is governed by N—H $\cdots$ O hydrogen bonding [1.94 (3) Å], along with several C—H $\cdots$ O interactions.

6. Synthesis and crystallization

The title compound was obtained by refluxing 2-[4-(2-methylpropyl)phenyl]propanehydrazide (0.01 mol) and 2-acetyl thiophene (0.01 mol) in ethanol (20 ml) by adding a catalytic amount of concentrated sulfuric acid for 1 h. The excess solvent was removed under reduced pressure. The solid product obtained was filtered, washed with ethanol, and dried. Single crystals suitable for X-ray analysis were obtained by slow evaporation from an ethanol solution with 80% yield and melting point 340–342 K.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were refined using a DFIX restraint to ensure chemically reasonable bond lengths and angles, with their $U_{\text{iso}}(\text{H})$ values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms.

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₂₄ N ₂ O ₂ S
M_r	328.46
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	7.9057 (3), 10.1929 (3), 12.2794 (3)
α, β, γ (°)	83.238 (1), 89.201 (1), 71.122 (1)
V (Å ³)	929.45 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	0.18
Crystal size (mm)	0.77 × 0.66 × 0.55
Data collection	
Diffractometer	Bruker D8 Quest Eco
Absorption correction	Multi-scan (SADABS, Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.874, 0.907
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27745, 4620, 4098
R_{int}	0.021
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.041, 0.123, 1.03
No. of reflections	4620
No. of parameters	304
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.25, −0.33

Computer programs: APEX2 and SAINT (Bruker 2012), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), ORTEP-3 for Windows and WinGX (Farrugia, 2012) and publCIF (Westrip, 2010).

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Computing details

2-[4-(2-Methylpropyl)phenyl]-*N'*-[(1*Z*)-1-(thiophen-2-yl)ethylidene]propanehydrazide

Crystal data

C₁₉H₂₄N₂OS

$M_r = 328.46$

Triclinic, *P*1

Hall symbol: -P 1

$a = 7.9057(3) \text{ \AA}$

$b = 10.1929(3) \text{ \AA}$

$c = 12.2794(3) \text{ \AA}$

$\alpha = 83.238(1)^\circ$

$\beta = 89.201(1)^\circ$

$\gamma = 71.122(1)^\circ$

$V = 929.45(5) \text{ \AA}^3$

$Z = 2$

$F(000) = 352$

$D_x = 1.174 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 27745 reflections

$\theta = 2.7\text{--}28.3^\circ$

$\mu = 0.18 \text{ mm}^{-1}$

$T = 293 \text{ K}$

BLOCK, white

$0.77 \times 0.66 \times 0.55 \text{ mm}$

Data collection

Bruker D8 Quest Eco

diffractometer

Graphite monochromator

ϕ and ω scans

Absorption correction: multi-scan
(SADABS, Krause *et al.*, 2015)

$T_{\min} = 0.874$, $T_{\max} = 0.907$

27745 measured reflections

4620 independent reflections

4098 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -10 \rightarrow 10$

$k = -13 \rightarrow 13$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.123$

$S = 1.03$

4620 reflections

304 parameters

0 restraints

0 constraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.1712P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.25 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.33 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
H7	0.214 (2)	1.0985 (18)	0.6861 (13)	0.061 (4)*
H11	−0.014 (2)	1.2611 (16)	0.7709 (12)	0.051 (4)*
H3	0.7134 (19)	1.3440 (16)	0.4536 (12)	0.050 (4)*
H10	0.538 (2)	1.4079 (17)	0.6116 (13)	0.061 (4)*
H4B	0.744 (2)	1.0670 (19)	0.5259 (14)	0.064 (4)*
H12B	−0.225 (3)	1.480 (2)	0.7002 (18)	0.093 (6)*
H6	0.487 (2)	1.0259 (18)	0.6006 (14)	0.064 (4)*
H9	0.267 (2)	1.4757 (18)	0.6996 (14)	0.066 (5)*
H4A	0.816 (2)	1.1609 (18)	0.5930 (15)	0.066 (5)*
H1A	0.603 (2)	1.173 (2)	0.3246 (15)	0.073 (5)*
H1C	0.468 (3)	1.291 (2)	0.3788 (16)	0.081 (6)*
H2B	0.929 (3)	1.263 (2)	0.3186 (18)	0.085 (6)*
H2C	1.001 (3)	1.205 (2)	0.438 (2)	0.102 (8)*
H12A	−0.118 (3)	1.413 (2)	0.6042 (19)	0.090 (6)*
H1B	0.591 (3)	1.327 (2)	0.2852 (18)	0.085 (6)*
H1	0.107 (2)	1.3514 (19)	1.0060 (15)	0.068 (5)*
H19	0.276 (3)	0.649 (2)	0.9227 (19)	0.099 (7)*
H12C	−0.080 (3)	1.536 (2)	0.6532 (18)	0.093 (7)*
H2A	0.940 (3)	1.108 (2)	0.3691 (17)	0.089 (6)*
H17	0.426 (3)	0.840 (2)	1.1552 (19)	0.087 (6)*
H15A	0.198 (4)	1.177 (3)	1.166 (2)	0.134 (10)*
H15B	0.342 (4)	1.212 (3)	1.113 (3)	0.140 (10)*
H15C	0.371 (4)	1.072 (3)	1.171 (2)	0.121 (9)*
H18	0.433 (3)	0.615 (2)	1.1025 (19)	0.100 (7)*
S1	0.20178 (5)	0.88866 (4)	0.90928 (3)	0.05992 (13)
N2	0.16268 (14)	1.17435 (11)	0.94142 (8)	0.0464 (2)
C8	0.20740 (16)	1.29536 (11)	0.69966 (9)	0.0410 (2)
N1	0.11506 (16)	1.31606 (11)	0.94519 (9)	0.0499 (2)
C6	0.4414 (2)	1.11989 (12)	0.61919 (10)	0.0515 (3)
O1	−0.01124 (18)	1.53227 (10)	0.86090 (8)	0.0697 (3)
C11	0.02513 (17)	1.34485 (13)	0.75071 (10)	0.0464 (3)
C9	0.30698 (17)	1.38476 (12)	0.67826 (11)	0.0481 (3)
C10	0.46957 (18)	1.34333 (12)	0.62781 (11)	0.0509 (3)
C5	0.54019 (17)	1.20942 (11)	0.59659 (9)	0.0452 (3)

C7	0.2783 (2)	1.16138 (13)	0.67006 (10)	0.0508 (3)
C16	0.27929 (17)	0.94374 (13)	1.02006 (10)	0.0493 (3)
C4	0.71791 (18)	1.16349 (13)	0.54132 (12)	0.0532 (3)
C14	0.24044 (16)	1.09260 (13)	1.02689 (10)	0.0471 (3)
C13	0.03963 (17)	1.40564 (13)	0.85616 (10)	0.0483 (3)
C3	0.73007 (17)	1.25536 (12)	0.43557 (11)	0.0504 (3)
C19	0.2924 (3)	0.71716 (17)	0.96246 (16)	0.0715 (4)
C15	0.2901 (3)	1.1379 (2)	1.13036 (14)	0.0667 (4)
C17	0.3711 (2)	0.83168 (17)	1.09363 (14)	0.0662 (4)
C1	0.5877 (2)	1.26297 (17)	0.35180 (13)	0.0626 (4)
C12	−0.1107 (2)	1.4535 (2)	0.67142 (15)	0.0662 (4)
C2	0.9153 (2)	1.20371 (19)	0.38798 (19)	0.0730 (5)
C18	0.3772 (3)	0.70272 (18)	1.05916 (17)	0.0793 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0657 (2)	0.0562 (2)	0.0589 (2)	−0.01866 (16)	0.00501 (16)	−0.01461 (15)
N2	0.0515 (5)	0.0443 (5)	0.0446 (5)	−0.0157 (4)	0.0091 (4)	−0.0100 (4)
C8	0.0512 (6)	0.0374 (5)	0.0349 (5)	−0.0146 (4)	0.0009 (4)	−0.0062 (4)
N1	0.0637 (6)	0.0459 (5)	0.0423 (5)	−0.0181 (5)	0.0081 (4)	−0.0131 (4)
C6	0.0726 (8)	0.0343 (5)	0.0478 (6)	−0.0158 (5)	0.0117 (6)	−0.0113 (4)
O1	0.1087 (9)	0.0434 (5)	0.0536 (5)	−0.0177 (5)	0.0126 (5)	−0.0136 (4)
C11	0.0506 (6)	0.0452 (6)	0.0464 (6)	−0.0183 (5)	0.0035 (5)	−0.0101 (5)
C9	0.0554 (7)	0.0323 (5)	0.0572 (7)	−0.0135 (5)	0.0081 (5)	−0.0107 (5)
C10	0.0545 (7)	0.0363 (5)	0.0632 (7)	−0.0163 (5)	0.0087 (6)	−0.0077 (5)
C5	0.0543 (6)	0.0348 (5)	0.0413 (5)	−0.0081 (4)	0.0028 (5)	−0.0019 (4)
C7	0.0706 (8)	0.0403 (6)	0.0494 (6)	−0.0263 (6)	0.0123 (6)	−0.0134 (5)
C16	0.0489 (6)	0.0508 (6)	0.0459 (6)	−0.0128 (5)	0.0103 (5)	−0.0078 (5)
C4	0.0526 (7)	0.0384 (6)	0.0581 (7)	−0.0022 (5)	0.0054 (5)	−0.0006 (5)
C14	0.0454 (6)	0.0516 (6)	0.0437 (6)	−0.0141 (5)	0.0089 (4)	−0.0098 (5)
C13	0.0564 (7)	0.0447 (6)	0.0460 (6)	−0.0176 (5)	0.0111 (5)	−0.0116 (5)
C3	0.0542 (7)	0.0345 (5)	0.0573 (7)	−0.0073 (5)	0.0124 (5)	−0.0062 (5)
C19	0.0836 (11)	0.0522 (8)	0.0815 (11)	−0.0230 (7)	0.0200 (9)	−0.0180 (7)
C15	0.0766 (10)	0.0660 (9)	0.0523 (8)	−0.0127 (8)	−0.0068 (7)	−0.0152 (7)
C17	0.0760 (10)	0.0569 (8)	0.0569 (8)	−0.0110 (7)	0.0005 (7)	−0.0022 (6)
C1	0.0711 (9)	0.0559 (8)	0.0540 (8)	−0.0124 (7)	0.0055 (7)	−0.0043 (6)
C12	0.0561 (8)	0.0679 (9)	0.0691 (9)	−0.0121 (7)	−0.0106 (7)	−0.0087 (8)
C2	0.0617 (9)	0.0606 (9)	0.0887 (12)	−0.0100 (7)	0.0251 (9)	−0.0085 (8)
C18	0.0958 (13)	0.0514 (8)	0.0786 (11)	−0.0105 (8)	0.0100 (9)	0.0008 (8)

Geometric parameters (Å, °)

S1—C19	1.7115 (18)	C4—C3	1.5300 (18)
S1—C16	1.7225 (14)	C4—H4B	0.978 (18)
N2—C14	1.2862 (16)	C4—H4A	1.003 (18)
N2—N1	1.3761 (14)	C14—C15	1.5005 (19)
C8—C9	1.3860 (17)	C3—C1	1.512 (2)

C8—C7	1.3881 (15)	C3—C2	1.521 (2)
C8—C11	1.5175 (17)	C3—H3	0.923 (15)
N1—C13	1.3473 (17)	C19—C18	1.341 (3)
N1—H1	0.859 (19)	C19—H19	0.93 (2)
C6—C5	1.3841 (18)	C15—H15A	0.85 (3)
C6—C7	1.3853 (19)	C15—H15B	0.97 (4)
C6—H6	0.962 (17)	C15—H15C	0.87 (3)
O1—C13	1.2297 (15)	C17—C18	1.414 (3)
C11—C13	1.5208 (17)	C17—H17	0.90 (2)
C11—C12	1.527 (2)	C1—H1A	0.98 (2)
C11—H11	1.002 (16)	C1—H1C	0.96 (2)
C9—C10	1.3793 (18)	C1—H1B	0.99 (2)
C9—H9	0.945 (17)	C12—H12B	0.93 (2)
C10—C5	1.3949 (16)	C12—H12A	0.98 (2)
C10—H10	0.979 (17)	C12—H12C	0.95 (2)
C5—C4	1.5087 (18)	C2—H2B	1.01 (2)
C7—H7	0.942 (18)	C2—H2C	0.92 (3)
C16—C17	1.373 (2)	C2—H2A	0.99 (2)
C16—C14	1.4599 (18)	C18—H18	0.96 (2)
C19—S1—C16	91.71 (8)	O1—C13—C11	121.97 (12)
C14—N2—N1	117.92 (10)	N1—C13—C11	117.84 (11)
C9—C8—C7	117.67 (11)	C1—C3—C2	110.69 (14)
C9—C8—C11	120.64 (10)	C1—C3—C4	111.69 (12)
C7—C8—C11	121.67 (11)	C2—C3—C4	110.71 (12)
C13—N1—N2	120.01 (10)	C1—C3—H3	108.8 (9)
C13—N1—H1	116.0 (12)	C2—C3—H3	107.3 (9)
N2—N1—H1	122.2 (12)	C4—C3—H3	107.4 (9)
C5—C6—C7	121.56 (11)	C18—C19—S1	112.06 (14)
C5—C6—H6	119.9 (10)	C18—C19—H19	130.0 (14)
C7—C6—H6	118.5 (10)	S1—C19—H19	118.0 (14)
C8—C11—C13	109.93 (10)	C14—C15—H15A	112 (2)
C8—C11—C12	111.19 (12)	C14—C15—H15B	110.5 (19)
C13—C11—C12	110.02 (11)	H15A—C15—H15B	102 (3)
C8—C11—H11	107.7 (8)	C14—C15—H15C	113.9 (18)
C13—C11—H11	107.3 (9)	H15A—C15—H15C	113 (3)
C12—C11—H11	110.6 (9)	H15B—C15—H15C	105 (2)
C10—C9—C8	121.41 (10)	C16—C17—C18	112.44 (16)
C10—C9—H9	117.7 (11)	C16—C17—H17	123.3 (14)
C8—C9—H9	120.9 (11)	C18—C17—H17	124.2 (14)
C9—C10—C5	121.13 (11)	C3—C1—H1A	113.0 (11)
C9—C10—H10	120.7 (9)	C3—C1—H1C	114.2 (12)
C5—C10—H10	118.1 (10)	H1A—C1—H1C	104.8 (16)
C6—C5—C10	117.32 (11)	C3—C1—H1B	111.6 (12)
C6—C5—C4	121.29 (11)	H1A—C1—H1B	104.6 (16)
C10—C5—C4	121.38 (11)	H1C—C1—H1B	108.0 (16)
C6—C7—C8	120.91 (11)	C11—C12—H12B	111.8 (14)
C6—C7—H7	120.5 (10)	C11—C12—H12A	108.8 (13)

C8—C7—H7	118.6 (10)	H12B—C12—H12A	107.1 (18)
C17—C16—C14	129.06 (13)	C11—C12—H12C	112.5 (14)
C17—C16—S1	110.69 (11)	H12B—C12—H12C	107.5 (18)
C14—C16—S1	120.23 (10)	H12A—C12—H12C	109.0 (19)
C5—C4—C3	114.56 (10)	C3—C2—H2B	112.8 (11)
C5—C4—H4B	109.1 (10)	C3—C2—H2C	110.4 (15)
C3—C4—H4B	109.4 (10)	H2B—C2—H2C	106.9 (19)
C5—C4—H4A	110.0 (10)	C3—C2—H2A	109.9 (12)
C3—C4—H4A	108.2 (10)	H2B—C2—H2A	107.1 (17)
H4B—C4—H4A	105.1 (13)	H2C—C2—H2A	109.6 (19)
N2—C14—C16	115.38 (11)	C19—C18—C17	113.10 (16)
N2—C14—C15	125.65 (13)	C19—C18—H18	124.1 (14)
C16—C14—C15	118.95 (12)	C17—C18—H18	122.7 (14)
O1—C13—N1	120.17 (12)		
C14—N2—N1—C13	177.41 (11)	N1—N2—C14—C16	176.95 (10)
C9—C8—C11—C13	−53.84 (15)	N1—N2—C14—C15	−2.2 (2)
C7—C8—C11—C13	127.93 (12)	C17—C16—C14—N2	175.00 (14)
C9—C8—C11—C12	68.24 (15)	S1—C16—C14—N2	−6.57 (15)
C7—C8—C11—C12	−109.99 (14)	C17—C16—C14—C15	−5.8 (2)
C7—C8—C9—C10	0.99 (19)	S1—C16—C14—C15	172.59 (12)
C11—C8—C9—C10	−177.31 (12)	N2—N1—C13—O1	176.36 (12)
C8—C9—C10—C5	−0.2 (2)	N2—N1—C13—C11	−5.30 (17)
C7—C6—C5—C10	0.43 (19)	C8—C11—C13—O1	103.88 (14)
C7—C6—C5—C4	179.90 (12)	C12—C11—C13—O1	−18.90 (18)
C9—C10—C5—C6	−0.56 (19)	C8—C11—C13—N1	−74.43 (14)
C9—C10—C5—C4	179.97 (12)	C12—C11—C13—N1	162.80 (13)
C5—C6—C7—C8	0.4 (2)	C5—C4—C3—C1	−57.96 (16)
C9—C8—C7—C6	−1.11 (19)	C5—C4—C3—C2	178.20 (14)
C11—C8—C7—C6	177.17 (12)	C16—S1—C19—C18	−0.08 (15)
C19—S1—C16—C17	0.06 (12)	C14—C16—C17—C18	178.51 (14)
C19—S1—C16—C14	−178.63 (11)	S1—C16—C17—C18	−0.04 (19)
C6—C5—C4—C3	123.70 (14)	S1—C19—C18—C17	0.1 (2)
C10—C5—C4—C3	−56.85 (18)	C16—C17—C18—C19	0.0 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O1 ⁱ	0.859 (18)	2.119 (18)	2.9537 (15)	163.6 (16)

Symmetry code: (i) $-x, -y+3, -z+2$.

Table 2. The energy values (eV) of global reactivity descriptors for the title compound.

Global reactivity Descriptors	Calculated values (eV)
E(HOMO)	−6.0826
E(LUMO)	−1.7796
Energy gap	4.303
Electron affinity (A)	1.7796

Ionisation energy (I)	6.0826
Electronegativity (χ)	3.9311
Chemical hardness (η)	2.1515
Chemical potential (μ)	-3.9311
Chemical hardness (S)	0.2324
Electrophilicity index (ω)	3.5913
