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N-Methyl-2-{3-methyl-2-[(2*Z*)-pent-2-en-1-yl]-cyclopent-2-en-1-ylidene}hydrazinecarbothioamide

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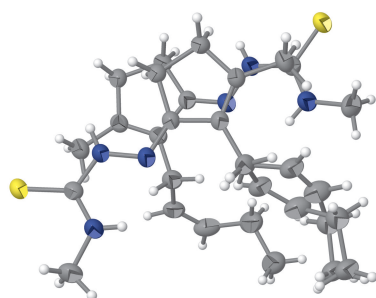
Keywords: thiosemicarbazone; *cis*-jasmone; methylthiosemicarbazone derivative; centrosymmetric dimers; crystal structure; Hirshfeld analysis.

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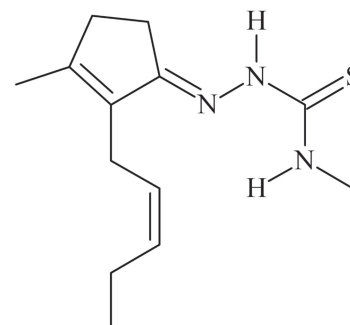
Structural data: full structural data are available from iucrdata.iucr.org

The equimolar and hydrochloric acid-catalysed reaction between *cis*-jasmone and 4-methylthiosemicarbazide in ethanolic solution yields the title compound, C₁₃H₂₁N₃S (common name: *cis*-jasmone 4-methylthiosemicarbazone). Two molecules with all atoms in general positions are present in the asymmetric unit. In one of them, the carbon chain is disordered [site occupancy ratio = 0.821 (3):0.179 (3)]. The thiosemicarbazone entities [N—N—C(=S)—N] are approximately planar, with the maximum deviation from the mean plane through the selected atoms being −0.0115 (16) Å (r.m.s.d. = 0.0078 Å) for the non-disordered molecule and 0.0052 (14) Å (r.m.s.d. = 0.0031 Å) for the disordered one. The molecules are not planar, since the jasmone groups have a chain with *sp*³-hybridized carbon atoms and, in addition, the thiosemicarbazone fragments are attached to the respective carbon five-membered rings and the dihedral angles between them for each molecule amount to 8.9 (1) and 6.3 (1)°. In the crystal, the molecules are connected through pairs of N—H...S and C—H...S interactions into crystallographically independent centrosymmetric dimers, in which rings of graph-set motifs *R*₂²(8) and *R*₂¹(7) are observed. A Hirshfeld surface analysis indicates that the major contributions for the crystal cohesion are from H...H (70.6%), H...S/S...H (16.7%), H...C/C...H (7.5%) and H...N/N...H (4.9%) interactions [considering the two crystallographically independent molecules and only the disordered atoms with the highest s.o.f. for the evaluation].

3D view



Chemical scheme



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Table 1

Selected geometric parameters ($\text{\AA}$, $^\circ$) for the two crystallographically independent *cis*-jasmone 4-methylthiosemicarbazone molecules, **JMTSC-1** and **JMTSC-2**.

Compound	Atom chain	Torsion angle	Atom chain	Torsion angle
JMTSC-1	N1/N2/C11/N3	-1.2 (3)	C5/C6/C7/C8	114.6 (3)
JMTSC-1	N1/N2/C11/S1	178.55 (17)	C7/C8/C9/C10	128.0 (4)
JMTSC-2	N4/N5/C25/N6	0.8 (3)	C18/C19/C20A/C21A	139.9 (4)
JMTSC-2	N4/N5/C25/S2	-179.57 (16)	C18/C19/C20B/C21B	-117.6 (13)
			C20A/C21A/C22A/C23A	121.9 (4)
			C20B/C21B/C22B/C23B	-95 (4)
	Fragment	Max. deviation ^a	r.m.s.d.	Angle ^b
JMTSC-1	N1/N2/C11/S1/N3	-0.0115 (16) [N2]	0.0078	
JMTSC-1	C1—C5 ring	0.0130 (16) [C4]	0.0089	8.9 (1)
JMTSC-2	N4/N5/C25/S2/N6	0.0052 (14) [N5]	0.0031	
JMTSC-2	C14—C18 ring	0.0078 (16) [C17]	0.0054	6.3 (1)
	Bond lengths ^c	N—N	N—C	C=S
JMTSC-1		1.392 (3)	1.351 (3)	1.680 (2)
JMTSC-2		1.394 (2)	1.357 (3)	1.678 (2)

Notes: (a) The maximum deviation from the mean plane through the selected atoms; (b) angle to previous plane; (c) bond lengths for the N1/N2/C11/S1 and N4/N5/C25/S2 entities.

Structure description

To the best of our knowledge, the first crystal structure of *cis*-jasmone thiosemicarbazone was reported recently and it was pointed out that this derivative based on non-substituted *cis*-jasmone shows antifungal activity (Orsoni *et al.*, 2020; Jamiołkowska *et al.*, 2022).

As part of our interest in thiosemicarbazones attached to natural product derivatives and on the influence of the substituent groups at the terminal N atom on the supra-molecular arrangement, we report here the synthesis, crystal structure and Hirshfeld analysis of *cis*-jasmone 4-methylthio-

semicarbazone. It is important to highlight that the substituents at the terminal N atom are relevant not only to the crystal packing, but also to the biological properties of the thiosemicarbazone derivatives. For example, a small chemical library of 4-methylthiosemicarbazones has been studied for the treatment of Parkinson's disease (Mathew *et al.*, 2021) and for microbial growth inhibition (D'Agostino *et al.*, 2022). In addition, for a review article on coordination compounds with 4-methylthiosemicarbazone derivatives including biological applications and catalytic activity, see: Monsur Showkot Hossain *et al.* (2023).

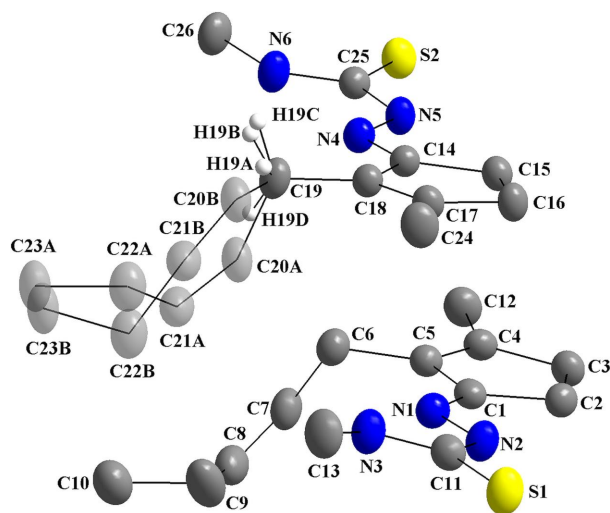


Figure 1

The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 40% probability level for the two crystallographically independent molecules. Disordered atoms are drawn with 40% transparency and labelled C20A, C21A, C22A, C23A, H19A and H19B [s.o.f. = 0.821 (3)] and C20B, C21B, C22B, C23B, H19C and H19D [s.o.f. = 0.179 (3)]. The remaining H atoms were omitted for clarity.

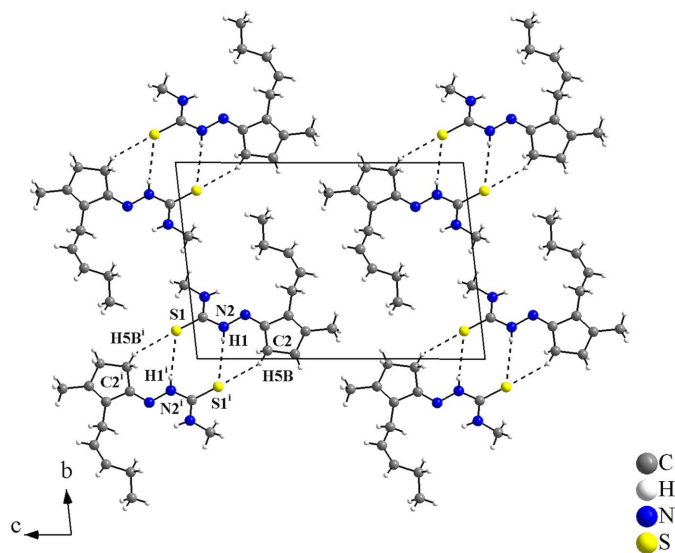


Figure 2

Crystal structure section of the title compound for the **JMTSC-1** molecule, showing the hydrogen-bond intermolecular interactions as dashed lines. The molecules are linked into centrosymmetric dimers *via* pairs of N—H...S and C—H...S interactions with graph-set motifs $R_2^2(8)$ and $R_1^2(7)$. [Symmetry code: (i) $-x, -y, -z + 2$.]

The asymmetric unit of the title compound comprises two molecules with all atoms in general positions, with one of them showing disorder over the carbon chain [site occupancy ratio = 0.821 (3):0.179 (3)]. The molecules are not planar due to the chain with sp^3 -hybridized carbon atoms in the jasmine fragment and the dihedral angles between the thiosemicarbazone fragment and the respective carbon five-membered ring, which amount to $8.9 (1)^\circ$ for the non-disordered molecule and $6.3 (1)^\circ$ for the disordered one (Fig. 1). To simplify the structure description, the non-disordered molecule, with atoms C1–C13/N–N3/S1, will be designated as **JMTSC-1**, while the disordered one, with the atoms C14–C23A/C23B/N4–N6/S2, will be designated as **JMTSC-2**. To get a stable refinement, the C20, C21, C22 and C23 atoms were split into two positions and *A*-labelled for the higher s.o.f and *B*-labelled for the lower. Atom C19, which is itself not disordered, is bound to C20*A* and C20*B*, and to achieve the best orientations for the C19–H bonds, the H19*A* and H19*B* atoms were also split, into two positions. Thus, the H19*A* and H19*B* atoms have a s.o.f. of 0.821 (3) and the H19*C* and H19*D* atoms have a s.o.f. of 0.179 (3). Selected geometric parameters for the structural description of **JMTSC-1** and **JMTSC-2** are given in Table 1; these are in agreement with literature data (Oliveira *et al.*, 2016; Rocha *et al.*, 2014).

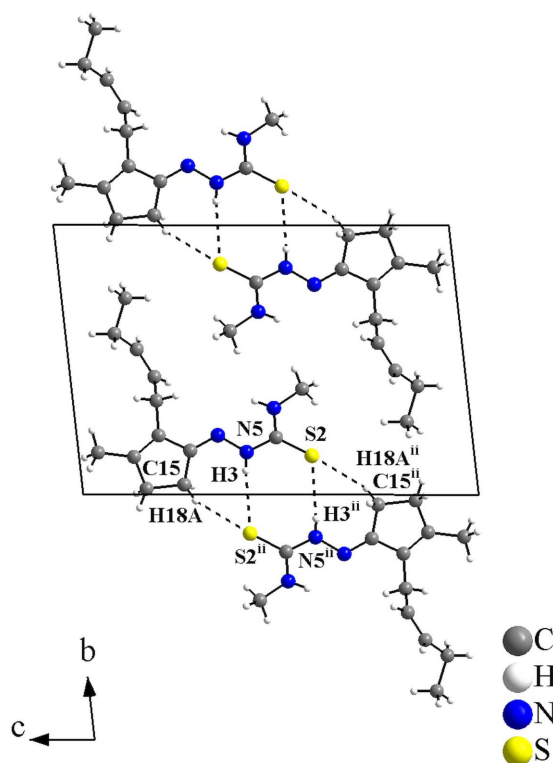


Figure 3

Crystal structure section of the title compound for the **JMTSC-2** molecule, showing the hydrogen-bonded intermolecular interactions drawn as dashed lines. Disorder is not shown for clarity. The molecules are linked into centrosymmetric dimers *via* pairs of N–H...S and C–H...S interactions with graph-set motifs $R_2^2(8)$ and $R_2^1(7)$. [Symmetry code: (ii) $-x + 1, -y, -z + 1$.]

Table 2

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H1...S1 ⁱ	0.81 (3)	2.80 (3)	3.591 (2)	167 (2)
C2–H5B...S1 ⁱ	0.97 (3)	2.90 (3)	3.457 (2)	117.4 (18)
N5–H3...S2 ⁱⁱ	0.84 (3)	2.75 (3)	3.585 (2)	172 (2)
C15–H18A...S2 ⁱⁱ	0.93 (2)	2.98 (2)	3.472 (2)	115.0 (17)

Symmetry codes: (i) $-x, -y, -z + 2$; (ii) $-x + 1, -y, -z + 1$.

For the supramolecular arrangement and Hirshfeld analysis, for clarity only the disordered atoms with the highest s.o.f. value were considered. In the crystal, the molecules are connected through pairs of N–H...S and C–H...S interactions into centrosymmetric dimers with graph-set motifs $R_2^2(8)$ and $R_2^1(7)$ (Table 2).

With the coordinates that were used for the refinement, the crystallographically independent dimers of the **JMTSC-1** molecules have the gravity centre located in the cell vertices (Fig. 2), and in the centre of the *ac* planes for the **JMTSC-2** molecules (Fig. 3). In addition, the molecules are stacked along [100] and only weak intermolecular interactions, *e.g.*, London dispersion forces can be presumed in this direction (Fig. 4).

The Hirshfeld surface analysis (Hirshfeld, 1977), the graphical representations and the two-dimensional Hirshfeld surface fingerprints (HSFP) were evaluated with the *Crystal Explorer* software (Wolff *et al.*, 2012). The Hirshfeld surface

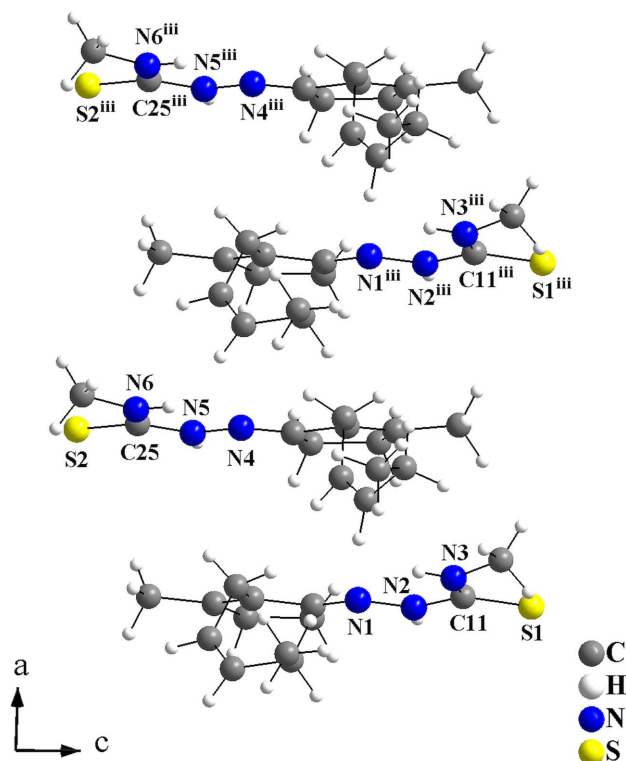


Figure 4

Selected crystal section of the title compound viewed along [010] showing the **JMTSC-1** and **JMTSC-2** molecules stacked along [100]. Only the non-H atoms of the thiosemicarbazone entities are labelled and disorder is not shown for clarity. [Symmetry code: (iii) $x + 1, y, z$.]

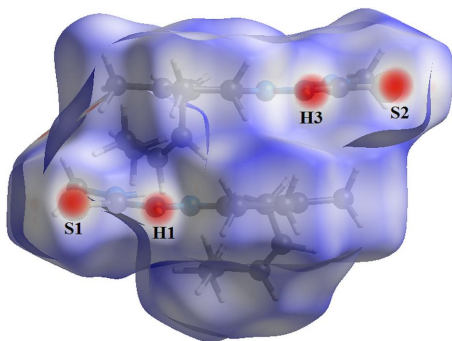


Figure 5

Hirshfeld surface graphical representation (d_{norm}) for the two crystallographically independent molecules of the title compound. The surface is drawn with transparency, and the disorder is not shown for clarity. The regions with strongest intermolecular interactions are shown in red (d_{norm} range: -0.216 to 1.522 a.u.).

analysis of the title compound, considering the **JMTSC-1** and the **JMTSC-2** molecules, suggests that the most relevant intermolecular interactions for the crystal packing are $\text{H}\cdots\text{H}$ (70.6%), $\text{H}\cdots\text{S}/\text{S}\cdots\text{H}$ (16.7%), $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ (7.5%) and $\text{H}\cdots\text{N}/\text{N}\cdots\text{H}$ (4.9%). A graphical representation of the Hirshfeld surface (d_{norm}) is shown in Fig. 5 with the locations of the strongest intermolecular contacts, *i.e.*, the regions around the atoms H1, H3, S1 and S2, indicated in red. These atoms are those involved in the $\text{H}\cdots\text{S}$ interactions showed in

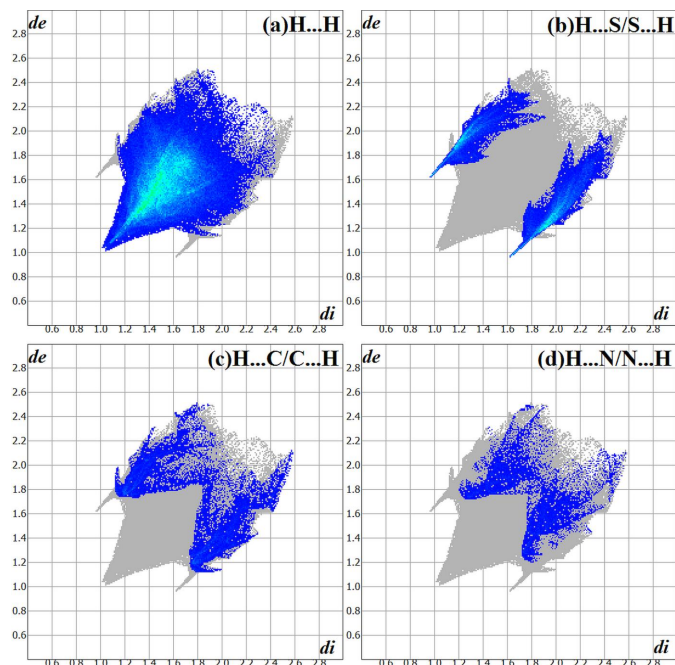


Figure 6

The Hirshfeld surface two-dimensional fingerprint plot for the title compound, showing the contacts in detail (cyan dots). The major contributions of the interactions to the crystal cohesion amount to (a) $\text{H}\cdots\text{H}$ (70.6%), (b) $\text{H}\cdots\text{S}/\text{S}\cdots\text{H}$ (16.7%), (c) $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ (7.5%) and (d) $\text{H}\cdots\text{N}/\text{N}\cdots\text{H}$ (4.9%). The d_i (x -axis) and the d_e (y -axis) values are the closest internal and external distances from given points on the Hirshfeld surface contacts (in Å). Regarding the disorder, only the atoms with the highest s.o.f. were considered.

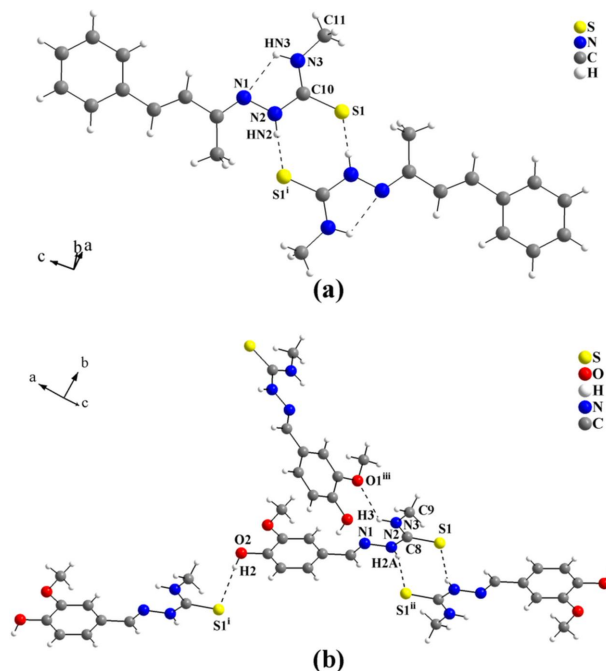


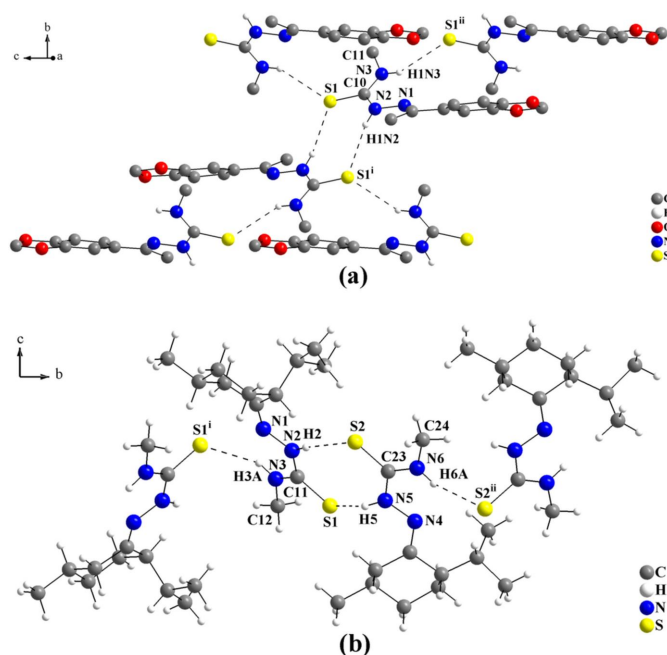
Figure 7

(a) Dimeric structure of the benzylideneacetone 4-methylthiosemicarbazone compound (Rocha *et al.*, 2014). The molecules are connected *via* pairs of centrosymmetric $\text{N}-\text{H}\cdots\text{S}$ interactions, with graph-set $R_2^2(8)$. [Symmetry code: (i) $-x+1, -y, -z$.] and (b) section of the molecular arrangement of the vanilline 4-methylthiosemicarbazone structure (Oliveira, Beck *et al.*, 2015). The molecules are connected by pairs of centrosymmetric $\text{N}-\text{H}\cdots\text{S}$ interactions, with graph-set $R_2^2(8)$. The dimers are linked further by $\text{O}-\text{H}\cdots\text{S}$ and $\text{N}-\text{H}\cdots\text{O}$ interactions into a tape-like structure. Only the subunit of the supramolecular arrangement is shown for clarity. [Symmetry codes: (i) $x+1, y-1, z$; (ii) $-x-2, -y, -z$; (iii) $-x-1, y+\frac{1}{2}, -z-\frac{1}{2}$.]

the previous figures (Figs. 2 and 3). The contributions to the crystal cohesion are shown as two-dimensional Hirshfeld surface fingerprint plots (HSFP) with cyan dots (Fig. 6).

The crystalline supramolecular arrangement of thiosemicarbazones depends on the template effect of the crystallization solvent, the presence of solvate molecules and on the crystallization methods. In addition, the steric effect of the substituents in the $R_1R_2\text{N}-\text{N}(\text{H})-\text{C}(=\text{S})-\text{NR}_3\text{R}_4$ fragment is of prime importance for the crystal packing. In the title compound, two structural features lead to the building of dimers. The first one is the terminal methyl group, $\text{N}(\text{H})\text{CH}_3$, which decreases the possibility for $\text{N}-\text{H}\cdots\text{S}$ intermolecular interactions and enhances the formation of hydrogen-bonded supramolecular structures. On the other side of the molecule, the second feature is the *cis*-jasmone entity, which, through steric hindrance, precludes intermolecular interactions, *e.g.*, $\text{N}-\text{H}\cdots\text{S}$ or $\text{N}-\text{H}\cdots\text{N}$ (Figs. 2 and 3); thus, four methyl-substituted thiosemicarbazone derivatives were selected for structural comparison with the title compound.

The first example is the crystal structure of benzylideneacetone 4-methylthiosemicarbazone (Rocha *et al.*, 2014). As a result of the steric effect of two methyl groups, one on the terminal N atom and other on the C atom attached to the thiosemicarbazone entity, dimer formation was favoured. The

**Figure 8**

(a) Section of the molecular arrangement of the 3',4'-(methylenedioxy)acetophenone 4-methylthiosemicarbazone structure (Oliveira, Näther *et al.*, 2015). The molecules are connected by pairs of centrosymmetric N—H...S interactions, with graph-set $R_2^2(8)$, and further linked by additional N—H...S interactions into a tape-like structure. H atoms were omitted for clarity and only the subunit of the supramolecular arrangement is shown [Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$] and (b) section of the molecular arrangement of the (-)-menthone 4-methylthiosemicarbazone structure (Oliveira *et al.*, 2016). The molecules are connected by pairs of N—H...S interactions, with graph-set $R_2^2(8)$, into non-centrosymmetric dimers and further linked by additional N—H...S interactions, forming a tape-like structure. Only the subunit of the supramolecular arrangement is shown for clarity [Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z + 1$; (ii) $-x + 2, y + \frac{1}{2}, -z + 1$.]

remaining N—H bond is involved in the N—H...N intramolecular interaction, with graph-set motif $S(5)$. Thus, the molecules are linked by N—H...S interactions, with graph-set motif $R_2^2(8)$, into centrosymmetric dimers. For the graphical representation of the dimeric unit, see Fig. 7(a).

The second selected molecule is the vanilline 4-methylthiosemicarbazone derivative (Oliveira, Beck *et al.*, 2015) in which the thiosemicarbazone entities are connected by N—H...S interactions, with graph-set motif $R_2^2(8)$, into centrosymmetric dimers. The dimers are further linked through N—H...S and O—H...S interactions and can be considered subunits of a hydrogen-bonded tape-like supramolecular arrangement. This is only possible because of the O atoms in the vanilline structure, see Fig. 7(b).

A further example is 3',4'-(methylenedioxy)acetophenone 4-methylthiosemicarbazone (Oliveira, Näther *et al.*, 2015). As mentioned above, the terminal methyl group decreases the dimensionality of the molecular arrangement and the thiosemicarbazone entities are connected by pairs of centrosymmetric N—H...S interactions, with graph-set motifs $R_2^2(8)$. A feature of the structural arrangement of this compound is that every thiosemicarbazone fragment bridges two other mol-

ecules through N—H...S interactions in opposite directions, see Fig. 8(a).

Finally, the structure of (-)-menthone 4-methylthiosemicarbazone (Oliveira *et al.*, 2016) shows a non-centrosymmetric dimer, with the molecules connected by pairs of N—H...S interactions, also with graph-set motif $R_2^2(8)$. A difference in this structure is the linking of the terminal N—H bonds between the molecules through N—H...S interactions into a tape-like structure. For the dimeric subunit of the supramolecular arrangement, see Fig. 8(b).

As observed for the title compound, pairs of N—H...S intermolecular interactions with graph-set motif $R_2^2(8)$ are a remarkable feature for the crystal structure of thiosemicarbazone derivatives. The supramolecular arrangement of the compounds depends on the structure of the substituents on the terminal N atom, as well as on the fragment attached to the first N atom.

Synthesis and crystallization

The starting materials are commercially available and were used without further purification. The synthesis of the *cis*-jasmane 4-methylthiosemicarbazone derivative was adapted from previously reported procedures (Oliveira, Beck *et al.*, 2015; Orsoni *et al.*, 2020). A mixture of ethanolic solutions of *cis*-jasmane (8 mmol in 50 ml) and 4-methylthiosemicarbazide (8 mmol in 50 ml) was catalysed with HCl and refluxed for 8 h. After cooling, the precipitated product was filtered off and washed with cold ethanol. Colourless single crystals suitable for X-ray diffraction were obtained from tetrahydrofuran by slow evaporation of the solvent at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. There are two crystallographically independent molecules in the asymmetric unit of the title compound and one of them, **JMTSC-2**, shows disorder over the chain of the *cis*-jasmane fragment, namely the C20, C21, C22, C23, H19C and H19D atoms (Fig. 1). These atoms were split over two positions, with the carbon atoms being *A*-labelled for the higher s.o.f. value positions and *B*-labelled for the lower [site-occupancy ratio = 0.821 (3):0.179 (3)]. The atom C19 is itself not disordered, but it is bound to C20A and C20B, and to get the best orientations for the C19—H bonds, the hydrogen atoms were disordered. Thus, H19A and H19B have the positions with higher s.o.f., while H19C and H19D have the positions with the lower. The EADP command was used to constrain the displacement parameters of the disordered carbon atoms.

The H atoms were treated by a mixture of constrained and independent refinement. The constrained H atoms were located in a difference-Fourier map, but were positioned with idealized geometry and refined using a riding model. For the C13H₃, C23AH₃, C23BH₃ and C26H₃ groups, the methyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$, and

the C—H bonds were set to 0.96 Å. In an analogous manner, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$, for the C22AH₂ and C22BH₂ groups the C—H bond lengths were set to 0.97 Å and for the C20AH, C20BH, C21AH and C21BH, were set to 0.93 Å. In addition, the C19—H bonds were set to 0.97 Å. The remaining H atoms were refined freely.

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Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₃ H ₂₁ N ₃ S
<i>M_r</i>	251.39
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	223
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.9583 (2), 11.2703 (2), 16.0080 (5)
α , β , γ (°)	83.0428 (18), 86.9392 (13), 76.5236 (18)
<i>V</i> (Å ³)	1385.51 (6)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.22
Crystal size (mm)	0.28 × 0.13 × 0.12
Data collection	
Diffractionmeter	Enraf–Nonius FR590 Kappa CCD
Absorption correction	Analytical (Alcock, 1970)
<i>T</i> _{min} , <i>T</i> _{max}	0.945, 0.978
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23118, 6319, 3700
<i>R</i> _{int}	0.056
(sin θ /λ) _{max} (Å ^{−1})	0.650
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.052, 0.140, 1.03
No. of reflections	6319
No. of parameters	432
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.29, −0.24

Computer programs: *COLLECT* (Nonius, 1998), *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SIR92* (Altomare *et al.*, 1994), *SHELXL2018/3* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006), *Crystal Explorer 3.1* (Wolff *et al.*, 2012), *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010) and *enCIFer* (Allen *et al.*, 2004).

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full crystallographic data

IUCrData (2024). **9**, x240013 [https://doi.org/10.1107/S2414314624000130]

***N*-Methyl-2-{3-methyl-2-[(2*Z*)-pent-2-en-1-yl]cyclopent-2-en-1-yl-idene}hydrazinecarbothioamide**

Adriano Bof de Oliveira, Leandro Bresolin, Johannes Beck and Jörg Daniels

N-Methyl-2-{3-methyl-2-[(2*Z*)-pent-2-en-1-yl]cyclopent-2-en-1-ylidene}hydrazinecarbothioamide

Crystal data

$C_{13}H_{21}N_3S$

$M_r = 251.39$

Triclinic, $P\bar{1}$

$a = 7.9583$ (2) Å

$b = 11.2703$ (2) Å

$c = 16.0080$ (5) Å

$\alpha = 83.0428$ (18)°

$\beta = 86.9392$ (13)°

$\gamma = 76.5236$ (18)°

$V = 1385.51$ (6) Å³

$Z = 4$

$F(000) = 544$

$D_x = 1.205$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 22795 reflections

$\theta = 2.9$ – 27.5 °

$\mu = 0.22$ mm⁻¹

$T = 223$ K

Prism, colourless

$0.28 \times 0.13 \times 0.12$ mm

Data collection

Enraf–Nonius FR590 Kappa CCD
diffractometer

Radiation source: sealed X-ray tube, Enraf
Nonius FR590

Horizontally mounted graphite crystal
monochromator

Detector resolution: 9 pixels mm⁻¹

CCD rotation images, thick slices, κ -goniostat
scans

Absorption correction: analytical
(Alcock, 1970)

$T_{\min} = 0.945$, $T_{\max} = 0.978$

23118 measured reflections

6319 independent reflections

3700 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.0$ °

$h = -10 \rightarrow 10$

$k = -14 \rightarrow 14$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.140$

$S = 1.03$

6319 reflections

432 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.4261P]$

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

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

$\Delta\rho_{\max} = 0.29$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ e Å⁻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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.0353 (3)	0.1677 (2)	0.75329 (13)	0.0349 (5)	
C2	0.0002 (4)	0.0424 (2)	0.75249 (14)	0.0389 (5)	
C3	0.0007 (4)	0.0248 (2)	0.65901 (15)	0.0417 (6)	
C4	0.0398 (3)	0.1401 (2)	0.61351 (13)	0.0376 (5)	
C5	0.0551 (3)	0.2205 (2)	0.66637 (13)	0.0364 (5)	
C6	0.0898 (4)	0.3467 (2)	0.64395 (17)	0.0442 (6)	
C7	−0.0620 (4)	0.4410 (2)	0.60830 (17)	0.0486 (6)	
H7	−0.090 (3)	0.427 (3)	0.5551 (18)	0.067 (9)*	
C8	−0.1493 (4)	0.5392 (3)	0.6422 (2)	0.0583 (7)	
H8	−0.243 (3)	0.593 (2)	0.6108 (16)	0.055 (7)*	
C9	−0.1227 (6)	0.5789 (3)	0.7249 (2)	0.0773 (10)	
H9A	−0.009 (5)	0.516 (4)	0.750 (2)	0.124 (14)*	
H9B	−0.226 (5)	0.571 (3)	0.762 (2)	0.110 (13)*	
C10	−0.1051 (5)	0.7098 (3)	0.7187 (2)	0.0664 (9)	
H10A	−0.003 (5)	0.725 (3)	0.684 (2)	0.090 (11)*	
H10B	−0.095 (5)	0.735 (3)	0.771 (2)	0.103 (13)*	
H10C	−0.203 (5)	0.764 (3)	0.692 (2)	0.102 (12)*	
C11	0.0650 (3)	0.2114 (2)	0.96479 (14)	0.0410 (6)	
C12	0.0594 (4)	0.1544 (3)	0.52013 (16)	0.0502 (7)	
C13	0.1722 (4)	0.3754 (3)	1.01676 (17)	0.0605 (8)	
H13A	0.078825	0.394161	1.057058	0.091*	
H13B	0.202888	0.449897	0.992591	0.091*	
H13C	0.270256	0.321649	1.044276	0.091*	
H1	0.000 (3)	0.099 (3)	0.9014 (16)	0.055 (9)*	
H2	0.136 (4)	0.342 (3)	0.9011 (18)	0.062 (9)*	
H4A	−0.107 (3)	0.012 (2)	0.6423 (14)	0.043 (7)*	
H4B	0.087 (3)	−0.043 (2)	0.6446 (14)	0.041 (6)*	
H5A	−0.111 (4)	0.036 (2)	0.7836 (16)	0.062 (8)*	
H5B	0.083 (3)	−0.023 (2)	0.7831 (16)	0.055 (7)*	
H6A	0.132 (3)	0.375 (2)	0.6918 (14)	0.037 (6)*	
H6B	0.178 (4)	0.344 (2)	0.6043 (17)	0.058 (8)*	
H11A	−0.050 (4)	0.144 (3)	0.4942 (19)	0.078 (10)*	
H11B	0.151 (4)	0.097 (3)	0.5017 (18)	0.070 (9)*	
H11C	0.082 (4)	0.233 (3)	0.4981 (18)	0.078 (10)*	
N1	0.0527 (2)	0.22380 (17)	0.81644 (11)	0.0402 (5)	
N2	0.0324 (3)	0.1628 (2)	0.89595 (12)	0.0443 (5)	
N3	0.1185 (3)	0.3154 (2)	0.95063 (14)	0.0503 (6)	
S1	0.03760 (10)	0.14256 (6)	1.06201 (4)	0.0555 (2)	
C14	0.5379 (3)	0.16267 (19)	0.71740 (13)	0.0329 (5)	

C15	0.5078 (4)	0.0367 (2)	0.74221 (14)	0.0370 (5)	
C16	0.5116 (4)	0.0211 (2)	0.83872 (14)	0.0412 (6)	
C17	0.5457 (3)	0.1391 (2)	0.86107 (13)	0.0375 (5)	
C18	0.5580 (3)	0.21881 (19)	0.79294 (13)	0.0347 (5)	
C19	0.5811 (3)	0.3483 (2)	0.78856 (15)	0.0448 (6)	
H19A	0.643811	0.356753	0.837003	0.054*	0.821 (3)
H19B	0.647894	0.366698	0.738193	0.054*	0.821 (3)
H19C	0.685443	0.350346	0.754772	0.054*	0.179 (3)
H19D	0.486229	0.399219	0.755824	0.054*	0.179 (3)
C20A	0.4087 (5)	0.4364 (3)	0.7871 (2)	0.0532 (8)	0.821 (3)
H20A	0.329480	0.415962	0.754005	0.064*	0.821 (3)
C21A	0.3451 (5)	0.5388 (3)	0.8238 (2)	0.0569 (9)	0.821 (3)
H21A	0.229448	0.576497	0.815022	0.068*	0.821 (3)
C22A	0.4385 (6)	0.5964 (3)	0.8758 (2)	0.0621 (10)	0.821 (3)
H22A	0.557592	0.550356	0.879680	0.075*	0.821 (3)
H22B	0.387225	0.595899	0.932190	0.075*	0.821 (3)
C23A	0.4333 (6)	0.7287 (3)	0.8386 (3)	0.0612 (11)	0.821 (3)
H23A	0.474681	0.729616	0.781112	0.092*	0.821 (3)
H23B	0.505314	0.763050	0.870457	0.092*	0.821 (3)
H23C	0.316591	0.776477	0.840756	0.092*	0.821 (3)
C20B	0.592 (2)	0.4084 (12)	0.8561 (9)	0.0532 (8)	0.179 (3)
H20B	0.682753	0.377545	0.892534	0.064*	0.179 (3)
C21B	0.479 (2)	0.5069 (15)	0.8714 (11)	0.0569 (9)	0.179 (3)
H21B	0.516842	0.521502	0.922436	0.068*	0.179 (3)
C22B	0.319 (3)	0.6156 (17)	0.8557 (11)	0.0621 (10)	0.179 (3)
H22C	0.239982	0.592198	0.820463	0.075*	0.179 (3)
H22D	0.260444	0.632136	0.909131	0.075*	0.179 (3)
C23B	0.366 (3)	0.728 (2)	0.8152 (14)	0.0612 (11)	0.179 (3)
H23D	0.363076	0.783573	0.856476	0.092*	0.179 (3)
H23E	0.284292	0.766305	0.772294	0.092*	0.179 (3)
H23F	0.479632	0.707879	0.790243	0.092*	0.179 (3)
C24	0.5633 (5)	0.1554 (3)	0.95104 (15)	0.0526 (7)	
C25	0.5613 (3)	0.2125 (2)	0.49665 (13)	0.0354 (5)	
C26	0.6433 (4)	0.3925 (2)	0.41676 (15)	0.0529 (7)	
H26A	0.739134	0.344372	0.387775	0.079*	
H26B	0.673244	0.465559	0.430318	0.079*	
H26C	0.544756	0.414694	0.381308	0.079*	
H3	0.508 (3)	0.089 (3)	0.5819 (16)	0.052 (8)*	
H4	0.611 (3)	0.348 (2)	0.5401 (16)	0.048 (7)*	
H17A	0.599 (3)	−0.050 (2)	0.8611 (15)	0.053 (7)*	
H17B	0.401 (3)	0.004 (2)	0.8647 (15)	0.050 (7)*	
H18A	0.590 (3)	−0.023 (2)	0.7182 (14)	0.044 (7)*	
H18B	0.398 (3)	0.032 (2)	0.7211 (15)	0.048 (7)*	
H24A	0.573 (4)	0.238 (3)	0.960 (2)	0.095 (11)*	
H24B	0.459 (4)	0.138 (3)	0.9862 (18)	0.070 (9)*	
H24C	0.662 (4)	0.096 (3)	0.9751 (19)	0.078 (10)*	
N4	0.5513 (2)	0.22004 (16)	0.64328 (11)	0.0370 (4)	
N5	0.5353 (3)	0.15779 (19)	0.57504 (11)	0.0384 (5)	

N6	0.6022 (3)	0.32130 (18)	0.49376 (13)	0.0453 (5)
S2	0.54338 (9)	0.14458 (6)	0.41094 (3)	0.04489 (19)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0328 (13)	0.0353 (12)	0.0357 (12)	−0.0050 (10)	−0.0016 (9)	−0.0056 (9)
C2	0.0442 (15)	0.0375 (13)	0.0337 (12)	−0.0094 (11)	0.0011 (11)	−0.0002 (10)
C3	0.0490 (16)	0.0385 (14)	0.0375 (13)	−0.0090 (12)	0.0019 (11)	−0.0076 (10)
C4	0.0383 (13)	0.0390 (13)	0.0335 (12)	−0.0059 (10)	0.0031 (10)	−0.0035 (9)
C5	0.0373 (13)	0.0366 (13)	0.0340 (12)	−0.0063 (10)	−0.0003 (9)	−0.0028 (9)
C6	0.0495 (16)	0.0426 (14)	0.0425 (15)	−0.0161 (12)	−0.0001 (13)	−0.0023 (11)
C7	0.0600 (18)	0.0396 (15)	0.0477 (16)	−0.0185 (13)	−0.0049 (13)	0.0053 (11)
C8	0.0541 (18)	0.0418 (16)	0.075 (2)	−0.0109 (13)	−0.0013 (15)	0.0083 (14)
C9	0.111 (3)	0.0500 (19)	0.064 (2)	−0.0098 (19)	0.033 (2)	−0.0092 (15)
C10	0.078 (2)	0.0518 (19)	0.067 (2)	−0.0093 (17)	0.0050 (19)	−0.0087 (15)
C11	0.0462 (15)	0.0418 (14)	0.0355 (13)	−0.0086 (11)	−0.0052 (10)	−0.0072 (10)
C12	0.063 (2)	0.0497 (17)	0.0366 (14)	−0.0105 (15)	0.0044 (13)	−0.0067 (12)
C13	0.083 (2)	0.0542 (17)	0.0518 (16)	−0.0235 (15)	−0.0136 (14)	−0.0132 (13)
N1	0.0460 (12)	0.0425 (11)	0.0324 (10)	−0.0114 (9)	−0.0009 (8)	−0.0029 (8)
N2	0.0604 (14)	0.0447 (13)	0.0321 (11)	−0.0210 (11)	−0.0027 (9)	−0.0035 (9)
N3	0.0715 (16)	0.0471 (13)	0.0372 (13)	−0.0233 (11)	−0.0059 (11)	−0.0036 (10)
S1	0.0842 (5)	0.0544 (4)	0.0327 (3)	−0.0261 (4)	−0.0033 (3)	−0.0034 (3)
C14	0.0371 (13)	0.0325 (12)	0.0292 (11)	−0.0085 (10)	0.0009 (9)	−0.0039 (9)
C15	0.0450 (15)	0.0325 (13)	0.0335 (12)	−0.0087 (11)	0.0003 (11)	−0.0045 (9)
C16	0.0585 (17)	0.0331 (13)	0.0319 (12)	−0.0119 (12)	0.0020 (12)	−0.0014 (9)
C17	0.0463 (14)	0.0353 (12)	0.0307 (12)	−0.0085 (10)	0.0020 (10)	−0.0064 (9)
C18	0.0404 (13)	0.0338 (12)	0.0315 (11)	−0.0110 (10)	0.0006 (9)	−0.0057 (9)
C19	0.0614 (17)	0.0410 (14)	0.0381 (13)	−0.0233 (12)	−0.0009 (11)	−0.0059 (10)
C20A	0.071 (2)	0.0345 (16)	0.0559 (19)	−0.0156 (15)	−0.0056 (16)	−0.0041 (13)
C21A	0.054 (2)	0.0441 (19)	0.072 (2)	−0.0135 (16)	−0.0031 (16)	−0.0019 (16)
C22A	0.089 (3)	0.052 (2)	0.049 (2)	−0.024 (2)	−0.004 (2)	−0.0035 (15)
C23A	0.092 (4)	0.0384 (17)	0.057 (3)	−0.023 (2)	−0.008 (2)	−0.0053 (17)
C20B	0.071 (2)	0.0345 (16)	0.0559 (19)	−0.0156 (15)	−0.0056 (16)	−0.0041 (13)
C21B	0.054 (2)	0.0441 (19)	0.072 (2)	−0.0135 (16)	−0.0031 (16)	−0.0019 (16)
C22B	0.089 (3)	0.052 (2)	0.049 (2)	−0.024 (2)	−0.004 (2)	−0.0035 (15)
C23B	0.092 (4)	0.0384 (17)	0.057 (3)	−0.023 (2)	−0.008 (2)	−0.0053 (17)
C24	0.079 (2)	0.0511 (18)	0.0284 (13)	−0.0152 (16)	−0.0032 (14)	−0.0050 (11)
C25	0.0385 (13)	0.0341 (12)	0.0324 (12)	−0.0075 (10)	0.0000 (9)	−0.0013 (9)
C26	0.0690 (18)	0.0466 (15)	0.0443 (14)	−0.0222 (13)	0.0037 (13)	0.0056 (11)
N4	0.0457 (12)	0.0375 (11)	0.0302 (10)	−0.0129 (9)	−0.0012 (8)	−0.0067 (8)
N5	0.0550 (13)	0.0338 (11)	0.0287 (10)	−0.0147 (10)	0.0006 (8)	−0.0044 (8)
N6	0.0667 (15)	0.0414 (12)	0.0314 (11)	−0.0209 (10)	0.0021 (10)	−0.0027 (9)
S2	0.0637 (4)	0.0434 (4)	0.0286 (3)	−0.0142 (3)	−0.0008 (3)	−0.0043 (2)

Geometric parameters (Å, °)

C1—N1	1.285 (3)	C16—H17A	0.98 (3)
C1—C5	1.461 (3)	C16—H17B	1.00 (3)
C1—C2	1.504 (3)	C17—C18	1.341 (3)
C2—C3	1.533 (3)	C17—C24	1.492 (3)
C2—H5A	1.00 (3)	C18—C19	1.506 (3)
C2—H5B	0.97 (3)	C19—C20B	1.359 (14)
C3—C4	1.500 (3)	C19—C20A	1.493 (4)
C3—H4A	0.96 (2)	C19—H19A	0.9700
C3—H4B	0.95 (2)	C19—H19B	0.9700
C4—C5	1.342 (3)	C19—H19C	0.9700
C4—C12	1.488 (3)	C19—H19D	0.9700
C5—C6	1.509 (3)	C20A—C21A	1.339 (5)
C6—C7	1.498 (4)	C20A—H20A	0.9300
C6—H6A	0.97 (2)	C21A—C22A	1.445 (5)
C6—H6B	0.92 (3)	C21A—H21A	0.9300
C7—C8	1.323 (4)	C22A—C23A	1.530 (5)
C7—H7	0.93 (3)	C22A—H22A	0.9700
C8—C9	1.488 (5)	C22A—H22B	0.9700
C8—H8	0.96 (3)	C23A—H23A	0.9600
C9—C10	1.505 (5)	C23A—H23B	0.9600
C9—H9A	1.07 (4)	C23A—H23C	0.9600
C9—H9B	1.00 (4)	C20B—C21B	1.29 (2)
C10—H10A	1.00 (4)	C20B—H20B	0.9300
C10—H10B	0.93 (4)	C21B—C22B	1.56 (3)
C10—H10C	0.96 (4)	C21B—H21B	0.9300
C11—N3	1.329 (3)	C22B—C23B	1.47 (3)
C11—N2	1.351 (3)	C22B—H22C	0.9700
C11—S1	1.680 (2)	C22B—H22D	0.9700
C12—H11A	1.02 (3)	C23B—H23D	0.9600
C12—H11B	0.91 (3)	C23B—H23E	0.9600
C12—H11C	0.96 (3)	C23B—H23F	0.9600
C13—N3	1.455 (3)	C24—H24A	0.97 (4)
C13—H13A	0.9600	C24—H24B	1.02 (3)
C13—H13B	0.9600	C24—H24C	0.97 (3)
C13—H13C	0.9600	C25—N6	1.335 (3)
N1—N2	1.392 (3)	C25—N5	1.357 (3)
N2—H1	0.81 (3)	C25—S2	1.678 (2)
N3—H2	0.83 (3)	C26—N6	1.453 (3)
C14—N4	1.292 (3)	C26—H26A	0.9600
C14—C18	1.463 (3)	C26—H26B	0.9600
C14—C15	1.498 (3)	C26—H26C	0.9600
C15—C16	1.535 (3)	N4—N5	1.394 (2)
C15—H18A	0.93 (2)	N5—H3	0.84 (3)
C15—H18B	0.97 (3)	N6—H4	0.85 (3)
C16—C17	1.505 (3)		

N1—C1—C5	122.2 (2)	C17—C16—H17B	112.7 (14)
N1—C1—C2	129.2 (2)	C15—C16—H17B	111.6 (14)
C5—C1—C2	108.56 (18)	H17A—C16—H17B	104 (2)
C1—C2—C3	104.79 (19)	C18—C17—C24	127.8 (2)
C1—C2—H5A	111.1 (15)	C18—C17—C16	112.35 (19)
C3—C2—H5A	113.8 (15)	C24—C17—C16	119.8 (2)
C1—C2—H5B	114.0 (16)	C17—C18—C14	109.11 (19)
C3—C2—H5B	111.5 (15)	C17—C18—C19	128.8 (2)
H5A—C2—H5B	102 (2)	C14—C18—C19	122.04 (19)
C4—C3—C2	104.5 (2)	C20B—C19—C18	125.2 (6)
C4—C3—H4A	111.7 (14)	C20A—C19—C18	109.9 (2)
C2—C3—H4A	112.7 (14)	C20A—C19—H19A	109.7
C4—C3—H4B	108.8 (14)	C18—C19—H19A	109.7
C2—C3—H4B	112.6 (14)	C20A—C19—H19B	109.7
H4A—C3—H4B	107 (2)	C18—C19—H19B	109.7
C5—C4—C12	127.4 (2)	H19A—C19—H19B	108.2
C5—C4—C3	112.30 (19)	C20B—C19—H19C	106.0
C12—C4—C3	120.3 (2)	C18—C19—H19C	106.0
C4—C5—C1	109.8 (2)	C20B—C19—H19D	106.0
C4—C5—C6	127.5 (2)	C18—C19—H19D	106.0
C1—C5—C6	122.7 (2)	H19C—C19—H19D	106.3
C7—C6—C5	114.0 (2)	C21A—C20A—C19	133.1 (3)
C7—C6—H6A	110.1 (13)	C21A—C20A—H20A	113.5
C5—C6—H6A	111.0 (13)	C19—C20A—H20A	113.5
C7—C6—H6B	107.0 (16)	C20A—C21A—C22A	126.4 (4)
C5—C6—H6B	110.0 (17)	C20A—C21A—H21A	116.8
H6A—C6—H6B	104 (2)	C22A—C21A—H21A	116.8
C8—C7—C6	127.3 (3)	C21A—C22A—C23A	110.4 (3)
C8—C7—H7	119.7 (17)	C21A—C22A—H22A	109.6
C6—C7—H7	112.9 (17)	C23A—C22A—H22A	109.6
C7—C8—C9	128.0 (3)	C21A—C22A—H22B	109.6
C7—C8—H8	117.7 (16)	C23A—C22A—H22B	109.6
C9—C8—H8	114.3 (15)	H22A—C22A—H22B	108.1
C8—C9—C10	113.3 (3)	C22A—C23A—H23A	109.5
C8—C9—H9A	106 (2)	C22A—C23A—H23B	109.5
C10—C9—H9A	112 (2)	H23A—C23A—H23B	109.5
C8—C9—H9B	107 (2)	C22A—C23A—H23C	109.5
C10—C9—H9B	109 (2)	H23A—C23A—H23C	109.5
H9A—C9—H9B	110 (3)	H23B—C23A—H23C	109.5
C9—C10—H10A	113.2 (19)	C21B—C20B—C19	122.2 (14)
C9—C10—H10B	113 (2)	C21B—C20B—H20B	118.9
H10A—C10—H10B	107 (3)	C19—C20B—H20B	118.9
C9—C10—H10C	110 (2)	C20B—C21B—C22B	157.0 (17)
H10A—C10—H10C	105 (3)	C20B—C21B—H21B	101.5
H10B—C10—H10C	108 (3)	C22B—C21B—H21B	101.5
N3—C11—N2	116.2 (2)	C23B—C22B—C21B	112.7 (18)
N3—C11—S1	122.86 (18)	C23B—C22B—H22C	109.0
N2—C11—S1	120.97 (19)	C21B—C22B—H22C	109.0

C4—C12—H11A	109.5 (17)	C23B—C22B—H22D	109.0
C4—C12—H11B	111.9 (18)	C21B—C22B—H22D	109.0
H11A—C12—H11B	108 (2)	H22C—C22B—H22D	107.8
C4—C12—H11C	112.6 (18)	C22B—C23B—H23D	109.5
H11A—C12—H11C	110 (2)	C22B—C23B—H23E	109.5
H11B—C12—H11C	105 (3)	H23D—C23B—H23E	109.5
N3—C13—H13A	109.5	C22B—C23B—H23F	109.5
N3—C13—H13B	109.5	H23D—C23B—H23F	109.5
H13A—C13—H13B	109.5	H23E—C23B—H23F	109.5
N3—C13—H13C	109.5	C17—C24—H24A	114 (2)
H13A—C13—H13C	109.5	C17—C24—H24B	110.5 (16)
H13B—C13—H13C	109.5	H24A—C24—H24B	108 (3)
C1—N1—N2	116.5 (2)	C17—C24—H24C	110.6 (18)
C11—N2—N1	119.4 (2)	H24A—C24—H24C	109 (3)
C11—N2—H1	119.8 (19)	H24B—C24—H24C	105 (2)
N1—N2—H1	120.8 (19)	N6—C25—N5	115.3 (2)
C11—N3—C13	123.6 (2)	N6—C25—S2	123.71 (17)
C11—N3—H2	118 (2)	N5—C25—S2	120.96 (17)
C13—N3—H2	118 (2)	N6—C26—H26A	109.5
N4—C14—C18	120.8 (2)	N6—C26—H26B	109.5
N4—C14—C15	129.58 (19)	H26A—C26—H26B	109.5
C18—C14—C15	109.57 (18)	N6—C26—H26C	109.5
C14—C15—C16	104.14 (19)	H26A—C26—H26C	109.5
C14—C15—H18A	112.0 (15)	H26B—C26—H26C	109.5
C16—C15—H18A	112.9 (14)	C14—N4—N5	116.71 (18)
C14—C15—H18B	109.4 (14)	C25—N5—N4	117.8 (2)
C16—C15—H18B	112.9 (14)	C25—N5—H3	120.8 (17)
H18A—C15—H18B	106 (2)	N4—N5—H3	121.4 (17)
C17—C16—C15	104.81 (19)	C25—N6—C26	124.3 (2)
C17—C16—H17A	111.6 (15)	C25—N6—H4	117.6 (17)
C15—C16—H17A	112.8 (14)	C26—N6—H4	118.0 (18)
N1—C1—C2—C3	−177.8 (2)	C15—C16—C17—C18	1.3 (3)
C5—C1—C2—C3	0.0 (3)	C15—C16—C17—C24	−178.2 (2)
C1—C2—C3—C4	1.2 (3)	C24—C17—C18—C14	178.0 (2)
C2—C3—C4—C5	−2.2 (3)	C16—C17—C18—C14	−1.4 (3)
C2—C3—C4—C12	177.1 (2)	C24—C17—C18—C19	−4.4 (4)
C12—C4—C5—C1	−176.9 (2)	C16—C17—C18—C19	176.2 (2)
C3—C4—C5—C1	2.3 (3)	N4—C14—C18—C17	−177.4 (2)
C12—C4—C5—C6	2.3 (4)	C15—C14—C18—C17	0.9 (3)
C3—C4—C5—C6	−178.5 (2)	N4—C14—C18—C19	4.8 (3)
N1—C1—C5—C4	176.6 (2)	C15—C14—C18—C19	−176.9 (2)
C2—C1—C5—C4	−1.4 (3)	C17—C18—C19—C20B	−0.8 (9)
N1—C1—C5—C6	−2.7 (3)	C14—C18—C19—C20B	176.5 (9)
C2—C1—C5—C6	179.3 (2)	C17—C18—C19—C20A	−91.4 (3)
C4—C5—C6—C7	73.9 (3)	C14—C18—C19—C20A	85.9 (3)
C1—C5—C6—C7	−107.0 (3)	C18—C19—C20A—C21A	139.9 (4)
C5—C6—C7—C8	114.6 (3)	C19—C20A—C21A—C22A	2.8 (6)

C6—C7—C8—C9	−2.1 (5)	C20A—C21A—C22A—C23A	121.9 (4)
C7—C8—C9—C10	128.0 (4)	C18—C19—C20B—C21B	−117.6 (13)
C5—C1—N1—N2	−179.33 (19)	C19—C20B—C21B—C22B	−4 (5)
C2—C1—N1—N2	−1.8 (4)	C20B—C21B—C22B—C23B	−95 (4)
N3—C11—N2—N1	−1.2 (3)	C18—C14—N4—N5	178.16 (19)
S1—C11—N2—N1	178.55 (17)	C15—C14—N4—N5	0.2 (4)
C1—N1—N2—C11	173.8 (2)	N6—C25—N5—N4	0.8 (3)
N2—C11—N3—C13	−175.1 (2)	S2—C25—N5—N4	−179.57 (16)
S1—C11—N3—C13	5.1 (4)	C14—N4—N5—C25	−175.3 (2)
N4—C14—C15—C16	178.1 (2)	N5—C25—N6—C26	176.9 (2)
C18—C14—C15—C16	−0.1 (3)	S2—C25—N6—C26	−2.7 (4)
C14—C15—C16—C17	−0.6 (3)		

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>
N2—H1 $\cdots$ S1 ⁱ	0.81 (3)	2.80 (3)	3.591 (2)	167 (2)
C2—H5B $\cdots$ S1 ⁱ	0.97 (3)	2.90 (3)	3.457 (2)	117.4 (18)
N5—H3 $\cdots$ S2 ⁱⁱ	0.84 (3)	2.75 (3)	3.585 (2)	172 (2)
C15—H18A $\cdots$ S2 ⁱⁱ	0.93 (2)	2.98 (2)	3.472 (2)	115.0 (17)

Symmetry codes: (i) $-x, -y, -z+2$; (ii) $-x+1, -y, -z+1$.