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## 1-(Thiophen-2-yl)ethanone thiosemicarbazone

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Key indicators: single-crystal X-ray study; T = 140 K; mean  $\sigma$ (C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.053; data-to-parameter ratio = 24.8.

The title compound,  $C_7H_9N_3S_2$ , crystallizes with two unique molecules in the unit cell, both present as thiosemicarbazide tautomers. The molecules differ principally in the dihedral angles between the thiophene ring planes and the planes through the non-H atoms of the hydrazinecarbothioamide units, viz. 9.80 (8)° for one molecule and 19.37 (7)° for the other. The hydrazinecarbothioamide units are reasonably planar, with r.m.s. deviations of 0.001Å for each of the molecules. In the crystal,  $N-H \cdot \cdot \cdot S$  hydrogen bonds link like molecules into  $R_2^2(8)$  inversion dimers. A three-dimensional network structure is generated by additional N-H···S hydrogen bonds and weak  $C-H \cdots S$  contacts between the unique molecules.

### **Related literature**

For related structures, see: Avsar et al. (2003); Arslan et al. (2004); Kusaï et al. (2009). For graph-set motifs, see: Bernstein et al. (1995). For the weighting scheme, see: Prince (1982); Watkin (1994).



#### **Experimental**

#### Crystal data

$C_7H_9N_3S_2$	$\gamma = 108.227 \ (8)^{\circ}$
$M_r = 199.31$	V = 925.52 (18) Å <sup>3</sup>
Triclinic, P1	Z = 4
a = 9.0037 (9)  Å	Mo $K\alpha$ radiation
b = 9.7800 (9)  Å	$\mu = 0.52 \text{ mm}^{-1}$
c = 12.1428 (12) Å	$T = 140 { m K}$
$\alpha = 104.575 \ (8)^{\circ}$	$0.50 \times 0.40 \times 0.30 \text{ mm}$
$\beta = 103.345 \ (8)^{\circ}$	

#### Data collection

Stoe IPDS diffractometer 13175 measured reflections 5386 independent reflections

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	217 parameters
$wR(F^2) = 0.053$	H-atom parameters constrained
S = 1.00	$\Delta \rho_{\rm max} = 0.40 \ {\rm e} \ {\rm \AA}^{-3}$
5373 reflections	$\Delta \rho_{\rm min} = -0.39 \text{ e } \text{\AA}^{-3}$

4634 reflections with  $I > 2\sigma(I)$ 

 $R_{\rm int} = 0.033$ 

### Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	$D-{\rm H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot$	$\cdot \cdot A$
$N1 - H11 \cdot \cdot \cdot S3^{i}$	0.83	2.56	3.3609 (16)	162	
$N21 - H212 \cdot \cdot \cdot S3^{ii}$	0.83	2.66	3.4691 (16)	167	
$N24 - H241 \cdots S23^{iii}$	0.85	2.77	3.6128 (14)	174	
$C7 - H72 \cdots S23^{ii}$	0.98	2.83	3.7236 (16)	153	
Symmetry codes: (i)	-x + 1, -y -	+2, -z+1;	(ii) $-x, -y+2,$	-z + 1;	(iii)
-x, -v + 2, -z					

Data collection: IPDS (Stoe & Cie, 1996); cell refinement: IPDS; data reduction: X-RED (Stoe & Cie 1996); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: CRYSTALS (Betteridge et al., 2003); molecular graphics: CAMERON (Watkin et al., 1996); software used to prepare material for publication: CRYSTALS.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2061).

#### References

Arslan, H., Flörke, U. & Külcü, N. (2004). Acta Chim. Slov. 51, 787-792.

Avsar, G., Arslan, H., Haupt, H.-J. & Külcü, N. (2003). Turk. J. Chem. 27, 281-285

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). Angew. Chem. Int. Ed. Engl. 34, 1555-1573
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). J. Appl. Cryst. 36, 1487.
- Kusaï, A., Mustayeen, A. K., Magali, A. & Gilles, B. (2009). Polyhedron, 29, 1273-1280.
- Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790.
- Prince, E. (1982). In Mathematical Techniques in Crystallography and Materials Scienc. New York: Springer-Verlag.
- Stoe & Cie (1996). IPDS Software and X-RED. Stoe & Cie, Darmstadt, Germany.
- Watkin, D. (1994). Acta Cryst. A50, 411-437.

Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). CAMERON. Chemical Crystallography Laboratory, Oxford, England.

supplementary materials

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## 1-(Thiophen-2-yl)ethanone thiosemicarbazone

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## Comment

NMR analysis of the title compound,  $(C_7H_9N_3S_2)_2$ , (see experimental) shows that two forms are present in solution with the thiosemicarbazide moiety being partially transformed into the thioenolsemicarbazide. The X-ray structure determination reveals that the compound crystallizes in the triclinic space group P-1 with two molecules in the asymmetric unit, both of which are present as the thiosemicarbazide tautomer. The molecular geometry is illustrated in Fig. 1. The C—S bond lengths 1.6921 (15) Å and 1.6884 (15) Å confirm the double bond character and are comparable to those observed for 1-(biphenyl-4-carbonyl)-3-*p*-tolyl-thiourea [1.647 (3) Å for C—S, 1.217 (3) and 1.224 (3) Å] (Avsar *et al.*, 2003). The C—N bond lengths are in the range [1.2920 (17) - 1.4122 (16) Å] which are shorter than normal single C—N bond lengths (Arslan *et al.*, 2004).

Both unique molecules form inversion related dimers with  $R^2_2(8)$  graph-set motifs (Bernstein *et al.*, 1995) through N1—H11···S3 and N24—H241···S23 hydrogen bonds. Unique molecules are further linked by N21—H212···S3 bonds supported by a weak C7—H72···S3 contacts which generate additional centrosymmetric  $R^2_2(11)$  motifs and a three dimensional network (Fig. 2).

## Experimental

2-Acetyl thiophene (1,2618 g, 10 mmol) was reacted with thiosemicarbazide (0.9114 g, 10 mmol) in CH<sub>3</sub>OH (50 ml) solution, to give the corresponding compound after one hour under reflux. After cooling to room temperature, a yellow solid was isolated and washed twice with diethyl ether. Yield: 79.5%. m.p. 142–146 °C. Anal. Calc. for C<sub>7</sub>H<sub>9</sub>N<sub>3</sub>S<sub>2</sub> (%): C, 42.19; H, 4.55; N, 21.08. Found: C, 42.22; H, 4.53; N, 21.01. Selected IR data (cm<sup>-1</sup>, KBr pellet): 3450, 3250 (v NH), 1630 (v C=N), 1160 (v C=S). <sup>1</sup>H NMR (200 MHz, CD<sub>6</sub>Cl,  $\delta$ , p.p.m.): 2.32 (s, 3H, –CH<sub>3</sub>); 7.42 (s, 2H, –NH<sub>2</sub>); 8.32 (s, 1H, –NH); 7.07–7.58 (m, 3H, C<sub>4</sub>H<sub>3</sub>S); 10.36 (s, 1H, SH);. <sup>13</sup>C NMR (200 MHz, CD<sub>3</sub>Cl,  $\delta$ , p.p.m.): 14.01 (–CH<sub>3</sub>); 68.09 (O––CH~2~); 70.12 (O– CH~2~); 127.12–143.152 (C<sub>4</sub>H<sub>3</sub>S); 145.30 (C=N); 178.02 (C=S). A CH<sub>3</sub>Cl solution of the title compound was mixed with ethanol (1/1). After several days, colorless block-shaped single crystals suitable for X-ray crystallographic analysis were obtained.

### Refinement

The H atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98, N—H in the range 0.86–0.89 N—H to 0.86 O—H = 0.82 Å) and  $U_{iso}$ (H) (in the range 1.2–1.5 times  $U_{eq}$  of the parent atom), after which the positions were refined with riding constraints.

Figures



Fig. 1. The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. Crystal packing of 1 viewed down the *b* axis. Hydrogen bonds are drawn as dashed lines.

## 1-(Thiophen-2-yl)ethanone thiosemicarbazone

Crystal data	
$C_7H_9N_3S_2$	Z = 4
$M_r = 199.31$	F(000) = 416
Triclinic, <i>P</i> Ī	$D_{\rm x} = 1.430 {\rm ~Mg~m}^{-3}$
Hall symbol: -P 1	Mo K $\alpha$ radiation, $\lambda = 0.71073$ Å
a = 9.0037 (9)  Å	Cell parameters from 0 reflections
b = 9.7800 (9)  Å	$\theta = 0-0^{\circ}$
c = 12.1428 (12)  Å	$\mu = 0.52 \text{ mm}^{-1}$
$\alpha = 104.575 \ (8)^{\circ}$	T = 140  K
$\beta = 103.345 \ (8)^{\circ}$	Parallelepiped, yellow
$\gamma = 108.227 \ (8)^{\circ}$	$0.50\times0.40\times0.30~mm$
$V = 925.52 (18) \text{ Å}^3$	
Data collection	
Stoe IPDS	$R_{int} = 0.033$
diffractometer	runt 0.055
graphite	$\theta_{\text{max}} = 30.9^\circ, \ \theta_{\text{min}} = 2.3^\circ$
ω scans	$h = -12 \rightarrow 12$
13175 measured reflections	$k = -12 \rightarrow 13$
5386 independent reflections	$l = -17 \rightarrow 17$
4634 reflections with $I > 2\sigma(I)$	

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.053$	Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982) [weight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) - A_{n-1}]*T_{n-1}(x)]$ where $A_i$ are the Chebychev coefficients listed be- low and $x = F /F$ max Method = Robust Weighting (Prince, 1982) W = [weight] * [1-(deltaF/6*sig-maF)^2]^2 A_i are: 17.0 19.0 6.62
S = 1.00	$(\Delta/\sigma)_{\text{max}} = 0.001$
5373 reflections	$\Delta \rho_{max} = 0.40 \text{ e} \text{ Å}^{-3}$
217 parameters	$\Delta \rho_{min} = -0.39 \text{ e } \text{\AA}^{-3}$
0 restraints	

## Special details

Experimental. Reflections affected by the beam-stop were not included in the refinement.

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
N1	0.26295 (15)	0.85450 (15)	0.42449 (11)	0.0287
C2	0.23744 (17)	0.93285 (17)	0.51896 (12)	0.0224
S3	0.37191 (5)	1.11020 (4)	0.61614 (4)	0.0264
N4	0.09273 (14)	0.86531 (14)	0.53590 (11)	0.0255
N5	-0.00908 (14)	0.71581 (14)	0.46373 (11)	0.0234
C6	-0.13491 (16)	0.65062 (17)	0.49325 (12)	0.0217
C7	-0.17662 (18)	0.72896 (18)	0.59706 (13)	0.0276
C8	-0.23815 (16)	0.49066 (17)	0.41921 (13)	0.0222
S9	-0.19349 (5)	0.39888 (5)	0.29754 (4)	0.0286
C10	-0.35441 (19)	0.22919 (18)	0.26747 (15)	0.0313
C11	-0.43840 (19)	0.24169 (18)	0.34678 (15)	0.0295
C12	-0.37117 (18)	0.39098 (17)	0.43411 (14)	0.0260
N21	-0.13026 (16)	0.79416 (16)	0.21760 (12)	0.0317
C22	-0.07537 (17)	0.87345 (17)	0.15117 (12)	0.0240
S23	-0.15386 (5)	0.99727 (5)	0.11278 (4)	0.0283
N24	0.05087 (15)	0.85422 (14)	0.11585 (11)	0.0245
N25	0.10126 (15)	0.74112 (14)	0.13786 (10)	0.0233
C26	0.22938 (17)	0.73180 (16)	0.11099 (12)	0.0213
C27	0.33339 (19)	0.83708 (19)	0.06322 (15)	0.0311
C28	0.27075 (17)	0.60356 (16)	0.12664 (12)	0.0210
S29	0.14366 (5)	0.46442 (5)	0.16514 (4)	0.0294
C30	0.2690 (2)	0.36424 (19)	0.15960 (14)	0.0324

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(A^2)$ 

# supplementary materials

C31	0.4021 (2)	0.43291 (19)	0.13032 (15)	0.0314
C32	0.40373 (19)	0.57103 (18)	0.11115 (14)	0.0282
H71	-0.2700	0.6650	0.6064	0.0418*
H73	-0.1962	0.8165	0.5899	0.0414*
H72	-0.0819	0.7680	0.6714	0.0395*
H101	-0.3781	0.1398	0.2028	0.0387*
H111	-0.5275	0.1609	0.3456	0.0342*
H121	-0.4131	0.4187	0.4973	0.0309*
H271	0.4474	0.8480	0.0869	0.0485*
H273	0.3333	0.9390	0.0904	0.0470*
H272	0.2894	0.8001	-0.0250	0.0484*
H301	0.2423	0.2727	0.1735	0.0391*
H311	0.4849	0.3958	0.1244	0.0388*
H321	0.4848	0.6364	0.0904	0.0338*
H41	0.0815	0.9026	0.6019	0.0329*
H241	0.0787	0.8967	0.0667	0.0309*
H12	0.1936	0.7641	0.3821	0.0374*
H211	-0.0889	0.7344	0.2366	0.0407*
H11	0.3561	0.8847	0.4174	0.0369*
H212	-0.2011	0.8090	0.2464	0.0402*

## Atomic displacement parameters $(Å^2)$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0205 (6)	0.0368 (7)	0.0220 (6)	0.0057 (5)	0.0103 (5)	0.0038 (5)
C2	0.0188 (6)	0.0292 (7)	0.0221 (6)	0.0107 (5)	0.0084 (5)	0.0108 (6)
S3	0.02314 (17)	0.02531 (17)	0.03061 (19)	0.00811 (14)	0.01403 (15)	0.00688 (15)
N4	0.0206 (6)	0.0279 (6)	0.0274 (6)	0.0080 (5)	0.0136 (5)	0.0058 (5)
N5	0.0191 (5)	0.0264 (6)	0.0245 (6)	0.0089 (5)	0.0085 (5)	0.0075 (5)
C6	0.0174 (6)	0.0298 (7)	0.0221 (6)	0.0116 (5)	0.0084 (5)	0.0114 (6)
C7	0.0236 (7)	0.0346 (8)	0.0257 (7)	0.0107 (6)	0.0129 (6)	0.0086 (6)
C8	0.0185 (6)	0.0293 (7)	0.0238 (7)	0.0125 (5)	0.0093 (5)	0.0115 (6)
S9	0.02536 (18)	0.03112 (19)	0.03085 (19)	0.01106 (15)	0.01547 (15)	0.00804 (15)
C10	0.0276 (7)	0.0267 (7)	0.0396 (9)	0.0120 (6)	0.0135 (7)	0.0079 (7)
C11	0.0253 (7)	0.0270 (7)	0.0417 (9)	0.0122 (6)	0.0152 (7)	0.0148 (7)
C12	0.0225 (7)	0.0309 (7)	0.0327 (8)	0.0136 (6)	0.0150 (6)	0.0152 (6)
N21	0.0333 (7)	0.0477 (8)	0.0356 (7)	0.0287 (6)	0.0220 (6)	0.0234 (6)
C22	0.0235 (7)	0.0300 (7)	0.0188 (6)	0.0144 (6)	0.0068 (5)	0.0044 (5)
S23	0.03127 (19)	0.0329 (2)	0.03109 (19)	0.02194 (16)	0.01527 (16)	0.01188 (16)
N24	0.0271 (6)	0.0323 (6)	0.0242 (6)	0.0197 (5)	0.0130 (5)	0.0119 (5)
N25	0.0249 (6)	0.0293 (6)	0.0210 (6)	0.0165 (5)	0.0091 (5)	0.0088 (5)
C26	0.0201 (6)	0.0269 (7)	0.0170 (6)	0.0114 (5)	0.0052 (5)	0.0059 (5)
C27	0.0293 (8)	0.0347 (8)	0.0405 (9)	0.0175 (7)	0.0173 (7)	0.0198 (7)
C28	0.0209 (6)	0.0259 (7)	0.0173 (6)	0.0109 (5)	0.0071 (5)	0.0066 (5)
S29	0.03128 (19)	0.0318 (2)	0.0328 (2)	0.01480 (16)	0.01744 (16)	0.01445 (16)
C30	0.0462 (9)	0.0327 (8)	0.0278 (7)	0.0228 (7)	0.0162 (7)	0.0134 (6)
C31	0.0376 (8)	0.0386 (9)	0.0317 (8)	0.0266 (7)	0.0163 (7)	0.0154 (7)
C32	0.0264 (7)	0.0351 (8)	0.0305 (8)	0.0177 (6)	0.0134 (6)	0.0128 (6)

Geometric parameters (Å, °)

N1—H12 $0.845$ N21—H211 $0.836$ N1—H11 $0.831$ N21—H212 $0.828$ C2—S3 $1.6921$ (15)C22—S23 $1.6884$ (15)C2—N4 $1.3528$ (17)N24—N25 $1.3525$ (17)N4—N5 $1.3754$ (17)N24—N25 $1.3811$ (16)N4—H41 $0.836$ N24—H241 $0.849$ N5—C6 $1.2920$ (17)N25—C26 $1.2923$ (17)C6—C7 $1.4931$ (19)C26—C27 $1.491$ (2)C6—C8 $1.455$ (2)C26—C28 $1.4586$ (19)C7—H71 $0.928$ C27—H271 $0.963$ C7—H72 $0.978$ C27—H272 $0.977$ C8—S9 $1.7270$ (14)C28—S29 $1.7243$ (14)C8—C12 $1.3696$ (19)C28—C32 $1.3719$ (18)S9—C10 $1.7127$ (16)S29—C30 $1.7122$ (16)C10—C11 $1.360$ (2)C30—C31 $1.351$ (2)C11—H101 $0.941$ C30—H301 $0.921$ C11—H111 $0.948$ C32—H211 $0.938$ C2—N1—H12 $119.3$ C22—N21—H211 $11.33$ C2—N1—H11 $119.4$ $1211-N21-H212$ $118.3$ N1—C2—N4 $11662$ (13) $N21-C22-N24$ $1200$ (11)C2—N4—H41 $119.2$ $N25-C26$ $11.672$ (12)N1—C2—N4 $119.99$ (12) $C22-N24-H211$ $12.2$ N4—N5-C6 $116.53$ (12) $N24-N25-C26$ $11.62$ (12)N5—C4 $119.09$ (12) $C22-N24-H214$ $12.297$ (11)N1—C2—N4 $119.99$ (12) $C22-N24-H214$ $12.297$ (11)<	N1—C2	1.3210 (17)	N21—C22	1.3249 (19)
N1-H110.831N21-H2120.828C2-S31.6921 (15)C22-S231.6884 (15)C2-N41.3528 (17)C22-N241.3525 (17)N4-N51.3754 (17)N24-N251.3811 (16)N4-H410.836N24-H2410.849N5-C61.2920 (17)N25-C261.2923 (17)C6-C71.4931 (19)C26-C271.491 (2)C6-C81.455 (2)C26-C271.491 (2)C7-H710.928C27-H2710.969C7-H720.978C27-H2720.977C8-S91.7270 (14)C28-S291.7743 (14)C9-C11.360 (2)C30-C311.351 (2)C10-C111.360 (2)C30-C311.351 (2)C10-C111.360 (2)C31-C321.424 (2)C11-C121.412 (2)C31-C321.424 (2)C11-H110.927C31-H3110.935C12-N1-H11119.5C22-N21-H211121.3C2-N1-H11119.5C22-N21-H212120.1H12-N1-H11119.4H21-N2-H212118.3N1-C2-S3124.09 (11)N21-C22-S23122.70 (11)N1-C2-N4116.62 (13)N21-C22-N24120.01 (11)C2-N4-M5119.09 (12)C22-N24-H24117.28 (13)S3-C2-N4119.28 (10)S3-C22-N24120.01 (11)C2-N4-M5119.09 (12)C22-N24-H241122.2N-M-C2-S3119.09 (12)C22-N24-H241122.2N-M-C4119.09 (12)C22-N24-H241123.13)S3-C2-N4<	N1—H12	0.845	N21—H211	0.836
C2=S3 $1.6921 (15)$ $C2=-S23$ $1.6884 (15)$ $C2=N4$ $1.3528 (17)$ $C2=N24$ $1.3525 (17)$ $N4=N5$ $1.3754 (17)$ $N24=N25$ $1.3811 (16)$ $N4=H41$ $0.836$ $N24=H241$ $0.849$ $N5=C6$ $1.2920 (17)$ $N25=C26$ $1.2923 (17)$ $C6=C7$ $1.4931 (19)$ $C26=C27$ $1.491 (2)$ $C6=C8$ $1.455 (2)$ $C26=C28$ $1.4586 (19)$ $C7=H71$ $0.928$ $C27=H271$ $0.963$ $C7=H73$ $0.947$ $C27=H272$ $0.977$ $C8=S9$ $1.7270 (14)$ $C28=C32$ $1.3719 (18)$ $S9=C10$ $1.7127 (16)$ $S29=C30$ $1.7122 (16)$ $C10=C11$ $1.360 (2)$ $C30=C31$ $1.351 (2)$ $C10=H101$ $0.941$ $C30=H301$ $0.921$ $C11=H111$ $0.927$ $C31=H311$ $0.938$ $C2=N1=H12$ $0.948$ $C3=H321$ $0.998$ $C2=N1=H11$ $119.3$ $C22=N21=H212$ $12.01$ $H12=N1=H11$ $119.4$ $H21=N2=N24$ $17.28 (13)$ $N1=C2=S3$ $12409 (11)$ $N21=C22=N24$ $12.70 (11)$ $N1=C2=N4$ $116.62 (13)$ $N21=C22=N24$ $12.70 (11)$ $N1=C2=N4$ $119.28 (10)$ $S23=C22=N24$ $117.62 (12)$ $N5=C6-C7$ $124.02 (13)$ $N25=C26-C27$ $12.58 (13)$ $N5=C4=T2$ $10.94$ $C22=N24=H241$ $12.70 (11)$ $C2=N4=H41$ $119.2$ $N25=C26-C27$ $12.58 (13)$ $N5=C6=C7$ $124.02 (13)$ $N25=C26-C27$	N1—H11	0.831	N21—H212	0.828
C2-N4 $1.3528$ (17) $C22-N24$ $1.3525$ (17) $N4-N5$ $1.3754$ (17) $N24-N25$ $1.3811$ (16) $N4-H41$ $0.836$ $N24-H241$ $0.849$ $N5-C6$ $1.2920$ (17) $N25-C26$ $1.2923$ (17) $C6-C7$ $1.4931$ (19) $C26-C27$ $1.491$ (2) $C6-C8$ $1.455$ (2) $C26-C28$ $1.4586$ (19) $C7-H71$ $0.928$ $C27-H271$ $0.963$ $C7-H72$ $0.978$ $C27-H272$ $0.977$ $C8-S9$ $1.7270$ (14) $C28-S29$ $1.7243$ (14) $C8-C12$ $1.3696$ (19) $C28-C32$ $1.7142$ (16) $C10-C11$ $1.360$ (2) $C30-C31$ $1.351$ (2) $C10-C11$ $0.941$ $C30-H301$ $0.921$ $C11-C12$ $1.412$ (2) $C31-C32$ $1.424$ (2) $C11-H11$ $0.927$ $C31-H311$ $0.938$ $C2-N1-H11$ $119.3$ $C22-N21-H211$ $121.3$ $C2-N1-H11$ $119.5$ $C22-N21-H212$ $120.1$ $N1-C2-S3$ $12409$ (11) $N21-C22-S23$ $12.70$ (11) $N1-C2-N4$ $119.62$ (13) $N21-C22-N24$ $120.01$ (11) $C2-N4-M51$ $119.62$ (13) <td>C2—S3</td> <td>1.6921 (15)</td> <td>C22—S23</td> <td>1.6884 (15)</td>	C2—S3	1.6921 (15)	C22—S23	1.6884 (15)
N4—N51.3754 (17)N24—N251.3811 (16)N4—H410.836N24—H2410.849N5—C61.2920 (17)N25—C261.2923 (17)C6—C71.4931 (19)C26—C271.491 (2)C6—C81.455 (2)C26—C281.4586 (19)C7—H170.928C27—H2710.963C7—H1730.947C27—H2730.969C7—H720.978C27—H2720.977C8—S91.7270 (14)C28—S291.7243 (14)C8—C121.3696 (19)C28—C321.3719 (18)S9—C101.7127 (16)S29—C301.712 (16)C10—C111.360 (2)C30—C311.351 (2)C10—H1010.941C30—H3010.921C11—C121.412 (2)C31—H3110.935C12—H1210.948C32—H3210.938C2—N1—H11119.5C22—N21—H21210.1H12—N1—H11119.4H21—N21—H212118.3N1—C2—S3124.09 (11)N21—C22—N24120.01N1—C2—N4116.62 (13)N21—C22—N24120.01N1—C2—N4119.28 (10)S23—C22—N24120.01N1—C2—N4119.28 (10)S23—C22—N24120.01N1—C2—N4119.87 (12)C22—N24—H241122.2V4—NS—C611.651 (12)N25—C26—C28118.29 (13)C3—C4—H41119.2N25—N24—H241122.2V4—NS—C611.651 (12)N25—C26—C28118.29 (13)S—C4—C12109.41271—C27—H271107.4C6—C7—H73112.7	C2—N4	1.3528 (17)	C22—N24	1.3525 (17)
N4—H41 $0.836$ N24—H241 $0.849$ N5—C61.2920 (17)N25—C261.2923 (17)C6—C71.4931 (19)C26—C271.491 (2)C6—C81.455 (2)C26—C281.4586 (19)C7—H710.928C27—H2710.963C7—H730.947C27—H2730.969C7—H720.978C27—H2720.977C8—S91.7270 (14)C28—S291.7243 (14)C8—C121.3696 (19)C28—C321.3719 (18)S9—C101.7127 (16)S29—C301.7122 (16)C10—C111.360 (2)C30—C311.351 (2)C10—H1010.941C30—H3010.921C11—C121.412 (2)C31—C321.424 (2)C11—C121.412 (2)C31—H3110.935C12—H110.927C31—H3110.935C12—N1—H12119.3C22—N21—H21212.13C2—N1—H11119.5C22—N21—H21212.13C2—N1—H11119.4H211—N21—H212118.3N1—C2—N4116.62 (13)N21—C22—N24120.01 (11)C2—N4—H41119.28N25—C24—N25118.70 (12)C2—N4—H41119.28N25—C24—N24117.62 (12)N5—N4—H41119.2N25—C24—C28115.93 (13)C2—N4—H41119.28C26—C27125.81 (13)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C7124.02 (13)N25—C26—C28115.93 (13)C7—C6—C8116.51 (12)N25—C26—C28115.93 (13)C6—C7—H73 </td <td>N4—N5</td> <td>1.3754 (17)</td> <td>N24—N25</td> <td>1.3811 (16)</td>	N4—N5	1.3754 (17)	N24—N25	1.3811 (16)
NS-C61.2920 (17)N25-C261.2923 (17)C6-C71.4931 (19)C26-C271.491 (2)C6-C81.455 (2)C26-C281.4586 (19)C7-H710.928C27-H2710.963C7-H720.977C27-H2730.969C7-H720.978C27-H2720.977C8-S91.7270 (14)C28-S291.7243 (14)C8-C121.3696 (19)C28-C321.3719 (18)S9-C101.7127 (16)S29-C301.7122 (16)C10-C111.360 (2)C30-C311.351 (2)C10-H1010.941C30-H3010.921C11-C121.412 (2)C31-C321.424 (2)C11-H1110.927C31-H3110.935C2-N1-H121.19.3C22-N21-H211121.3C2-N1-H11119.5C22-N21-H21218.3N1-C2-S3124.09 (11)N21-C22-S23122.70 (11)N1-C2-N4116.62 (13)N21-C22-N24117.28 (13)S3-C2-N4119.28 (10)S23-C22-N24117.28 (13)S3-C2-N4119.29 (10)S23-C22-N24117.28 (13)C2-N4-H41118.7C22-N24-H241117.28 (13)N5-C6-C7124.02 (13)N25-C26-C27125.81 (13)N5-C6-C7124.02 (13)N25-C26-C28115.93 (13)C7-C6-C8116.51 (12)N25-C26-C28115.93 (13)C6-C7-H73112.7C26-C27-H27311.6N5-C6-C7124.02 (13)N25-C26-C28115.93 (13)C6-C7-H73112.7C26-C27-H27311.6	N4—H41	0.836	N24—H241	0.849
C6-C7 $1.491(19)$ $C26-C27$ $1.491(2)$ $C6-C8$ $1.455(2)$ $C26-C28$ $1.458(19)$ $C7-H71$ $0.928$ $C27-H271$ $0.963$ $C7-H73$ $0.947$ $C27-H272$ $0.977$ $C8-S9$ $1.7270(14)$ $C28-S29$ $1.7243(14)$ $C8-C12$ $1.3696(19)$ $C28-C32$ $1.3719(18)$ $S9-C10$ $1.7127(16)$ $S29-C30$ $1.7122(16)$ $C10-C11$ $1.360(2)$ $C30-C31$ $1.351(2)$ $C10-H101$ $0.941$ $C30-H301$ $0.921$ $C11-H111$ $0.927$ $C31-H311$ $0.938$ $C2-N1-H12$ $0.948$ $C32-H321$ $0.938$ $C2-N1-H12$ $0.944$ $C32-H321$ $0.938$ $C2-N1-H12$ $0.948$ $C32-H121$ $0.938$ $C2-N1-H11$ $1.9.5$ $C22-N21-H211$ $121.3$ $C2-N1-H11$ $1.9.4$ $H21-N21-H212$ $120.1$ $H12-N1-H11$ $119.4$ $H21-N21-H212$ $183$ $N1-C2-S3$ $124.09(11)$ $N21-C22-N24$ $117.28(13)$ $S3-C2-N4$ $119.28(10)$ $S23-C22-N24$ $120.01(11)$ $C2-N4-H41$ $118.7$ $C22-N24-H241$ $122.2$ $N4-N5-C6$ $116.53(12)$ $N24-N25-C26$ $118.70(12)$ $C2-N4-H41$ $118.7$ $C22-N24-H241$ $122.2$ $N4-N5-C6$ $116.53(12)$ $N24-N25-C26$ $117.62(12)$ $N5-C6-C7$ $124.02(13)$ $N25-C26-C27$ $125.81(13)$ $N5-C6-C7-H73$ $112.7$ $C26-C7-H273$ $11.6$ $N1-N5-C6$	N5—C6	1.2920 (17)	N25—C26	1.2923 (17)
C6-C8 $1.455$ (2) $C26-C28$ $1.4586$ (19) $C7-H71$ $0.928$ $C27-H271$ $0.963$ $C7-H72$ $0.977$ $C27-H272$ $0.977$ $C8-S9$ $1.7270$ (14) $C28-S29$ $1.7243$ (14) $C8-S9$ $1.7270$ (14) $C28-S29$ $1.7243$ (14) $C8-C12$ $1.3696$ (19) $C28-C32$ $1.3719$ (18) $S9-C10$ $1.7127$ (16) $S29-C30$ $1.7122$ (16) $C10-C11$ $1.360$ (2) $C30-C31$ $0.921$ $C1-C12$ $1.412$ (2) $C31-C32$ $1.424$ (2) $C11-H11$ $0.941$ $C30-H301$ $0.921$ $C1-H12$ $0.948$ $C32-H321$ $0.938$ $C2-N1-H10$ $0.944$ $C32-N21-H211$ $21.3$ $C2-N1-H11$ $119.3$ $C22-N21-H211$ $21.3$ $C2-N1-H11$ $119.5$ $C22-N21-H212$ $120.1$ $112-N1-H11$ $119.4$ $H21-N21-H212$ $118.3$ $N1-C2-S3$ $124.09$ (11) $N21-C22-S23$ $122.70$ (11) $N1-C2-N4$ $116.62$ (13) $N21-C22-N24$ $120.01$ (11) $C2-N4-M5$ $119.09$ (12) $C22-N24-H241$ $17.32$ $C2-N4-M5$ $119.09$ (12) $N25-C26-C27$ $128.70$ (12) $C2-N4-M5$ $119.99$ (12) $N25-C26-C28$ $115.99$ (13) $C2-N4-M5$ $119.97$ (12) $N25-C26-C28$ $115.93$ (13) $C2-N4-M5$ $119.87$ (12) $N25-C26-C28$ $115.93$ (13) $C2-N4-M5$ $119.87$ (12) $C27-H272$ $10.7$ $N5-C6-C7$ $124.02$ (13) $N25-C2$	C6—C7	1.4931 (19)	C26—C27	1.491 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C8	1.455 (2)	C26—C28	1.4586 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7—Н71	0.928	С27—Н271	0.963
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7—Н73	0.947	С27—Н273	0.969
C8—S91.7270 (14)C28—S291.7243 (14)C8—C121.3696 (19)C28—C321.3719 (18)S9—C101.7127 (16)S29—C301.7122 (16)C10—C111.360 (2)C30—C311.351 (2)C10—H1010.941C30—H3010.921C11—C121.412 (2)C31—C321.424 (2)C11—H110.927C31—H3110.935C12—H1210.948C32—H3210.938C2—N1—H12119.3C22—N21—H211121.3C2—N1—H11119.5C22—N21—H212120.1H12—N1—H11119.4H211—N21—H212118.3N1—C2—S3124.09 (11)N21—C22—S23122.70 (11)N1—C2—N4116.62 (13)N21—C22—N24120.01 (11)C2—N4—H41118.7C22—N24—H241120.1N5—N4—H41119.28 (10)S23—C22—N24120.01 (11)C2—N4—H41118.7C22—N24—H241117.3N5—N4—H41119.2N25—N24—H241122.2N4—NS=C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C7124.02 (13)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H73112.7C26—C27—H273111.6M11—C7—H73107.4C26—C27—H273111.6M71—C7—H72109.4C26—C27—H272107.9M71—C7—H72109.4C26—C27—H272107.9M71—C7—H72109.4H271—C7—H27210	С7—Н72	0.978	С27—Н272	0.977
C8-C121.3696 (19)C28-C321.3719 (18)S9-C101.7127 (16)S29-C301.7122 (16)C10-C111.360 (2)C30-C311.351 (2)C10-H1010.941C30-H3010.921C11-C121.412 (2)C31-C321.424 (2)C11-H110.927C31-H3110.935C12-H1210.948C32-H3210.938C2-N1-H12119.3C22-N21-H211121.3C2-N1-H11119.5C22-N21-H212120.1H12-N1-H11119.4H211-N21-H212118.3N1-C2-S3124.09 (11)N21-C22-S23122.70 (11)N1-C2-N4116.62 (13)N21-C22-N24117.28 (13)S3-C2-N4119.09 (12)C22-N24-H241117.28 (13)C2-N4-N5119.09 (12)C22-N24-H241117.3N5-N4-H41118.7C22-N24-H241122.2N4-N5-C6116.53 (12)N24-N25-C26117.62 (12)N5-C6-C7124.02 (13)N25-C26-C27125.81 (13)N5-C6-C8116.11 (12)N25-C26-C28115.93 (13)C7-C6-C8119.87 (12)C27-C26-C28118.24 (12)C6-C7-H71112.8C26-C27-H271112.9C6-C7-H73112.7C26-C27-H273107.4C6-C7-H73107.0H271-C27-H272106.7H71-C7-H73107.0H271-C27-H272107.9H73-C7-H72109.4C26-C27-H272110.7H71-C7-H73107.0H271-C27-H272106.0C6-C8-S9120.53 (10)C26-C28-S29 <td>C8—S9</td> <td>1.7270 (14)</td> <td>C28—S29</td> <td>1.7243 (14)</td>	C8—S9	1.7270 (14)	C28—S29	1.7243 (14)
S9—C101.7127 (16)S29—C301.7122 (16)C10—C111.360 (2)C30—C311.351 (2)C10—H1010.941C30—H3010.921C11—C121.412 (2)C31—C321.424 (2)C11—H110.927C31—H3110.935C12—H1210.948C32—H3210.938C2—N1—H12119.3C22—N21—H212120.1H12_N1—H11119.5C22_N21—H21218.3N1—C2—S3124.09 (11)N21—C22—S23122.70 (11)N1—C2—N4116.62 (13)N21—C22—N24117.28 (13)S3—C2—N4119.99 (12)C22_N24—N25118.70 (12)C2—N4—M5119.09 (12)C22_N24—H24117.2C2—N4—H41119.2N25—N24—H24117.2N5—N4—H41119.2N25—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C28118.29 (13)N5—C6—C8116.11 (12)N25—C26—C28118.24 (12)C6—C7—H73112.7C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28118.24 (12)C6—C7—H73112.7C26—C27125.81 (13)N5—C6—C8110.71112.8C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7=H72109.4H271—C27—H272106.0C6—C7=H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28	C8—C12	1.3696 (19)	C28—C32	1.3719 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S9—C10	1.7127 (16)	S29—C30	1.7122 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10—C11	1.360 (2)	C30—C31	1.351 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10—H101	0.941	C30—H301	0.921
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—C12	1.412 (2)	C31—C32	1.424 (2)
C12—H1210.948C32—H3210.938C2—N1—H12119.3C22—N21—H211121.3C2—N1—H11119.5C22—N21—H212120.1H12—N1—H11119.4H211—N21—H212118.3N1—C2—S3124.09 (11)N21—C22—S23122.70 (11)N1—C2—N4116.62 (13)N21—C22—N24117.28 (13)S3—C2—N4119.28 (10)S23—C22—N24120.01 (11)C2—N4—N5119.09 (12)C22—N24—H25118.70 (12)C2—N4—H41118.7C22—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4H271—C27—H272107.9H71—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—S9120.53 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C11—H111	0.927	С31—Н311	0.935
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С12—Н121	0.948	C32—H321	0.938
C2N1H11119.5C22N21H212120.1H12N1H11119.4H211N21H212118.3N1C2S3124.09 (11)N21C22S23122.70 (11)N1C2N4116.62 (13)N21C22N24117.28 (13)S3C2N4119.28 (10)S23C22N24120.01 (11)C2N4N5119.09 (12)C22N24N25118.70 (12)C2N4H41118.7C22N24H241122.2N4N5C6116.53 (12)N24N25C26117.62 (12)N5C6C7124.02 (13)N25C26C27125.81 (13)N5C6C8116.11 (12)N25C26C28115.93 (13)C7C6C8119.87 (12)C27C26C28118.24 (12)C6C7H71112.8C26C27H271112.9C6C7H73107.0H271C27H273107.4C6C7H72109.4C26C27H272107.9H73C7H72105.1H273C27H272106.0C6C8S9120.53 (10)C26C28S29121.16 (10)C6C8C12128.75 (13)C26C28C32128.13 (13)S9C8C1210.66 (11)S29C28C3210.68 (11)	C2—N1—H12	119.3	C22—N21—H211	121.3
H12—N1—H11119.4H211—N21—H212118.3N1—C2—S3124.09 (11)N21—C22—S23122.70 (11)N1—C2—N4116.62 (13)N21—C22—N24117.28 (13)S3—C2—N4119.28 (10) $S23$ —C22—N24120.01 (11)C2—N4—N5119.09 (12)C22—N24—N25118.70 (12)C2—N4—H41118.7C22—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272100.7H71—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C2—N1—H11	119.5	C22—N21—H212	120.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H12—N1—H11	119.4	H211—N21—H212	118.3
N1—C2—N4116.62 (13)N21—C22—N24117.28 (13)S3—C2—N4119.28 (10)S23—C22—N24120.01 (11)C2—N4—N5119.09 (12)C22—N24—N25118.70 (12)C2—N4—H41118.7C22—N24—H241117.3N5—N4—H41119.2N25—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	N1—C2—S3	124.09 (11)	N21—C22—S23	122.70 (11)
S3—C2—N4119.28 (10)S23—C22—N24120.01 (11)C2—N4—N5119.09 (12)C22—N24—N25118.70 (12)C2—N4—H41118.7C22—N24—H241117.3N5—N4—H41119.2N25—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	N1—C2—N4	116.62 (13)	N21—C22—N24	117.28 (13)
C2N4N5119.09 (12)C22N24N25118.70 (12)C2N4H41118.7C22N24H241117.3N5N4H41119.2N25N24H241122.2N4N5C6116.53 (12)N24N25C26117.62 (12)N5C6C7124.02 (13)N25C26C27125.81 (13)N5C6C8116.11 (12)N25C26C28115.93 (13)C7C6C8119.87 (12)C27C26C28118.24 (12)C6C7H71112.8C26C27H271112.9C6C7H73112.7C26C27H273111.6H71C7H73107.0H271C27H273107.4C6C7H72109.4C26C27H272107.9H73C7H72105.1H273C27H272106.0C6C8S9120.53 (10)C26C28S29121.16 (10)C6C8C12128.75 (13)C26C28C32128.13 (13)S9C8C12110.66 (11)S29C28C32110.68 (11)	S3—C2—N4	119.28 (10)	S23—C22—N24	120.01 (11)
C2—N4—H41118.7C22—N24—H241117.3N5—N4—H41119.2N25—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272100.7H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C2—N4—N5	119.09 (12)	C22—N24—N25	118.70 (12)
N5—N4—H41119.2N25—N24—H241122.2N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C2—N4—H41	118.7	C22—N24—H241	117.3
N4—N5—C6116.53 (12)N24—N25—C26117.62 (12)N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	N5—N4—H41	119.2	N25—N24—H241	122.2
N5—C6—C7124.02 (13)N25—C26—C27125.81 (13)N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H73—C7—H72105.1H273—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	N4—N5—C6	116.53 (12)	N24—N25—C26	117.62 (12)
N5—C6—C8116.11 (12)N25—C26—C28115.93 (13)C7—C6—C8119.87 (12)C27—C26—C28118.24 (12)C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	N5—C6—C7	124.02 (13)	N25—C26—C27	125.81 (13)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N5—C6—C8	116.11 (12)	N25—C26—C28	115.93 (13)
C6—C7—H71112.8C26—C27—H271112.9C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C7—C6—C8	119.87 (12)	C27—C26—C28	118.24 (12)
C6—C7—H73112.7C26—C27—H273111.6H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	С6—С7—Н71	112.8	С26—С27—Н271	112.9
H71—C7—H73107.0H271—C27—H273107.4C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	С6—С7—Н73	112.7	С26—С27—Н273	111.6
C6—C7—H72109.4C26—C27—H272110.7H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	Н71—С7—Н73	107.0	H271—C27—H273	107.4
H71—C7—H72109.4H271—C27—H272107.9H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	С6—С7—Н72	109.4	C26—C27—H272	110.7
H73—C7—H72105.1H273—C27—H272106.0C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	H71—C7—H72	109.4	H271—C27—H272	107.9
C6—C8—S9120.53 (10)C26—C28—S29121.16 (10)C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	Н73—С7—Н72	105.1	H273—C27—H272	106.0
C6—C8—C12128.75 (13)C26—C28—C32128.13 (13)S9—C8—C12110.66 (11)S29—C28—C32110.68 (11)	C6—C8—S9	120.53 (10)	C26—C28—S29	121.16 (10)
S9—C8—C12         110.66 (11)         S29—C28—C32         110.68 (11)	C6—C8—C12	128.75 (13)	C26—C28—C32	128.13 (13)
	S9—C8—C12	110.66 (11)	S29—C28—C32	110.68 (11)
C8—S9—C10 91.72 (8) C28—S29—C30 91.80 (8)	C8—S9—C10	91.72 (8)	C28—S29—C30	91.80 (8)
S9—C10—C11 112.09 (12) S29—C30—C31 112.44 (12)	S9—C10—C11	112.09 (12)	S29—C30—C31	112.44 (12)
S9—C10—H101 121.9 S29—C30—H301 121.1	S9—C10—H101	121.9	S29—C30—H301	121.1

# supplementary materials

C11-C10-H101	126.1	С31—С30—Н301		126.4
C10-C11-C12	112.29 (14)	C30—C31—C32		112.12 (14)
C10-C11-H111	124.1	С30—С31—Н311		124.5
C12—C11—H111	123.6	С32—С31—Н311		123.4
C11—C12—C8	113.24 (13)	C31—C32—C28		112.97 (14)
C11—C12—H121	123.2	С31—С32—Н321		126.0
C8—C12—H121	123.5	С28—С32—Н321		121.0
Hydrogen-bond geometry (Å, °)				
D—H···A	D—H	H···A	$D \cdots A$	D—H··· $A$
N1—H11····S3 <sup>i</sup>	0.83	2.56	3.3609 (16)	162
N21—H212····83 <sup>ii</sup>	0.83	2.66	3.4691 (16)	167
N24—H241…S23 <sup>iii</sup>	0.85	2.77	3.6128 (14)	174
C7—H72···S23 <sup>ii</sup>	0.98	2.83	3.7236 (16)	153
Symmetry codes: (i) – <i>x</i> +1, – <i>y</i> +2, – <i>z</i> +1;	(ii) $-x$ , $-y+2$ , $-z+1$ ; (iii) $-x$	x, -y+2, -z.		





