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Synthesis and crystal structure of (*E*)-2-benzyl-1,3-diphenylisothiouronium iodide

Sungmin Kang,[a] Taek Hyeon Kim[a]‡ and Chee-Hun Kwak[b]*

[a]School of Chemical Engineering, College of Engineering, Chonnam National, University, Gwangju, 61186, South Korea, and [b]Department of Chemistry Education, Sunchon National University, 255 Jungang-ro, Sunchon, 57922, South Korea. *Correspondence e-mail: chkwak@sunchon.ac.kr

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‡ Additional correspondence author, email: thkim@jnu.ac.kr.

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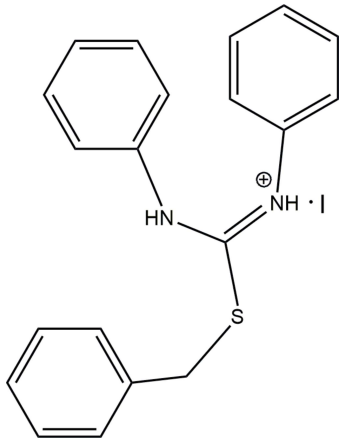
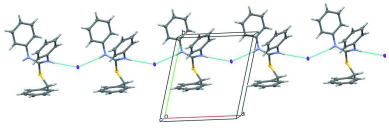
In the title molecular salt, $C_{20}H_{19}N_2S^+\cdot I^-$, prepared by the reaction of 1,3-diphenylthiourea and benzyl iodide, the C—S—C thioether bond angle is 101.66 (9)° and electrons are delocalized over the N$^+$═ C—N skeleton. The dihedral angle between the aromatic rings attached to the N atoms is 40.60 (9)°. In the crystal, N—H···I hydrogen bonds link the components into [100] chains.

1. Chemical context

Isothiouronium salts containing an *R*–S–C–(NH*R*)$_2^+$ moiety have been investigated as their hydrogen–bonding motifs for molecular recognition of anions (Yeo & Hong, 1998; Kubo *et al.*, 2000; Kato *et al.*, 2004; Nguyen *et al.*, 2009; Nguyen & Kim, 2010) and as organocatalysts (Nguyen & Kim, 2011, 2012; Lee *et al.*, 2018; Kang *et al.*, 2019). The isothiouronium group could enhance the acidity of their NH groups compared with thiourea and therefore be used as prospective alternative for thiourea. In addition, the chemical modification of the isothiouronium skeleton is readily performed using alkylation reactions of thiourea. As part of our work in this area, the synthesis and single-crystal structure of the title molecular salt, $C_{20}H_{19}N_2S^+\cdot I^-$ are reported herein.





2. Structural commentary

The title compound, $C_{20}H_{19}N_2S^+\cdot I^-$ (Fig. 1), is a molecular salt that arose from the reaction of 1,3-diphenylthiourea and benzyl iodide. There are three benzene rings, C1–C6 (I), C9–C14 (II) and C15–C20 (III) in the cation and the dihedral angles I/II, II/III and I/III are 50.36 (8), 40.60 (9) and

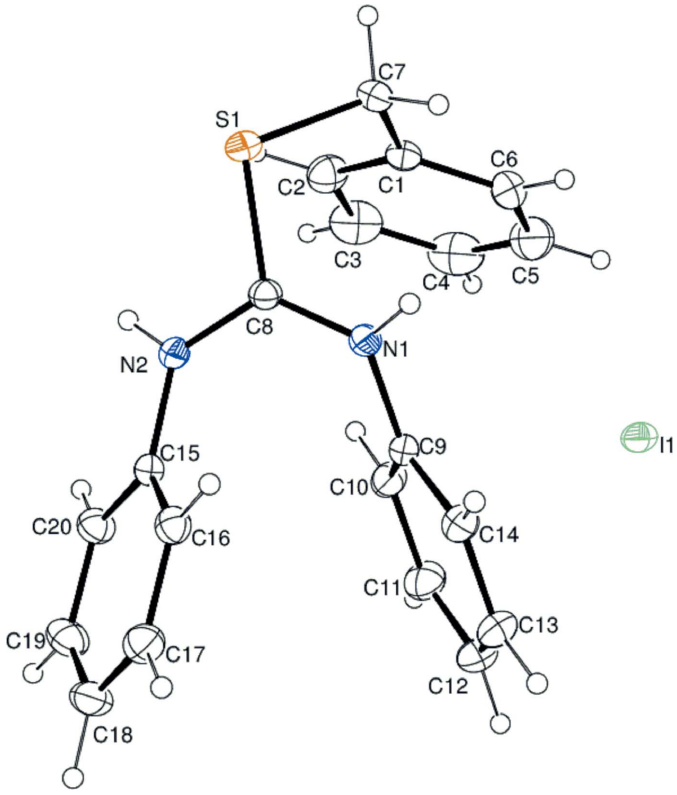


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at at the 30% probability level.

85.45 (9)°, respectively. In the cation, the *N*-[(phenylamino)-methylene]benzenaminium and toluyl units are linked to the sulfur atom as a thioether. The C7—S1 and C8—S1 bond lengths are 1.823 (2) and 1.751 (2) Å, respectively, and the C—S—C bond angle is 101.66 (9)°. The conformation of C1 and C8 about the C7—S1 bond is *gauche* [C1—C7—S1—C8 = 49.53 (16)°]. The C—S—C bond angle in the title compound is somewhat smaller than that for di-*p*-tolyl sulfide (109°; Blackmore & Abrahams, 1955) or the angle (107.8°) in oligomeric [ArCOArSArCOAr] (Ar = 1,4-phenylene; Colquhoun *et al.*, 1999) in which the aromatic rings are nearly coplanar. Rather, it is closer to that seen in diethyl sulfide [99.05 (4)°; Iijima *et al.*, 1977]. This result can be explained by the large dihedral angle between the benzene rings in the title compound. In the *N*-[(phenylamino)methylene]benzenaminium moiety of the title cation, the π-electrons of the iminium double bond are delocalized over the N1—C6—N2 skeleton [the C8—N1 and C8—N2 bond distances are 1.319 (2) and 1.332 (2) Å, respectively, and N1—C8—N2 = 124.53 (16)°].

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···I1^{i}	0.80 (3)	2.69 (3)	3.4781 (17)	171 (2)
N2—H2*N*···I1^{ii}	0.80 (3)	2.73 (3)	3.5242 (17)	169 (2)

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

3. Supramolecular features

In the crystal, the cations and anions are linked by almost linear N—H···I hydrogen bonds (Fig. 2, Table 1), generating [100] chains of alternating cations and anions, with adjacent species in the chain related by simple translation. No significant aromatic π–π stacking interactions occur, the shortest centroid–centroid separation being greater than 4.7 Å.

4. Database survey

A search of the Cambridge Structural Database (CSD, *via* CCDC Access Structures, November 2021; Groom *et al.*, 2016) resulted in 30 structures using isothiouronium as the keyword: 26 of them have a thioether skeleton. No results were found for 2-benzyl-1,3-diphenylisothiouronium or *N*-[(phenylamino)methylene]benzenaminium but the compound most similar to the title compound is *S*-benzylisothiouronium chloride (Barker & Powell, 1998). The bond angles of the thioether group in the *S*-benzylisothiouronium salts similar to

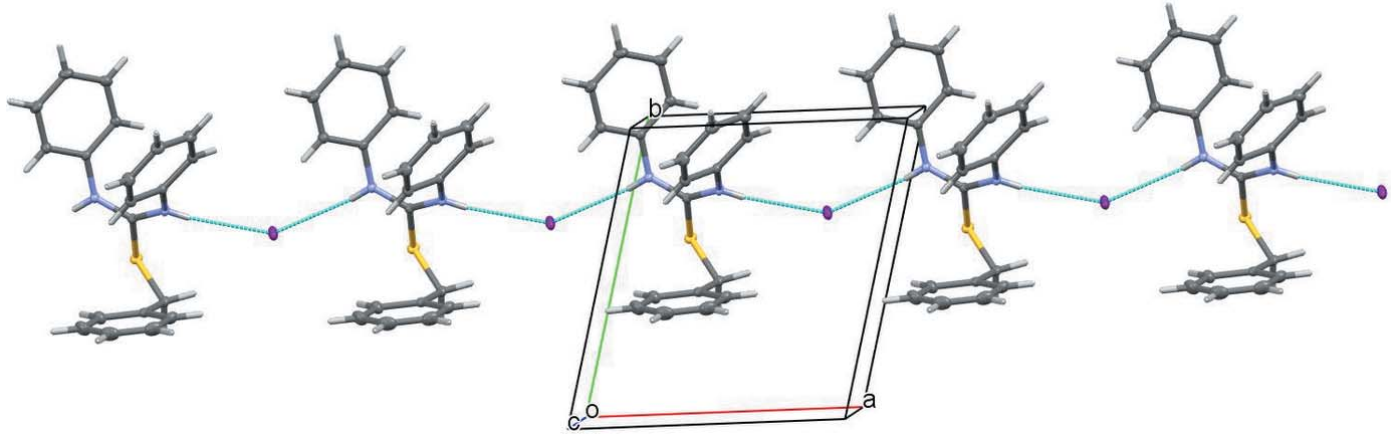


Figure 2
A view of a fragment of the [100] chain arising from N—H···I hydrogen bonds.

the title compound are the range 102.6 to 104.8°, depending on the counter-anions (Hemalatha & Veeravazhuthi, 2008; Ishii *et al.*, 2000; Pope & Boeyens, 1975).

5. Synthesis and crystallization

1,3-Diphenylthiourea (4.4 mmol) was added to a solution of benzyl iodide (13.2 mmol) in dry dichloromethane at room temperature. The reaction mixture was then stirred for 24 h and concentrated *in vacuo*. The residue was purified *via* flash chromatography (hexane:ethyl acetate = 8:2), to give the title compound as a yellow solid (1.14 g, yield 58%). A solution of isothiouronium iodide in methanol was slowly evaporated at room temperature to give crystals of the title compound: m.p. 442–443 K; ^{1}H NMR (300 MHz, DMSO): δ 7.21–7.39 (*m*, 15 H), δ 4.45 (*s*, 2 H); HR TOF–MS for $C_{20}H_{18}N_2S$: calculated 318.1186 (M^+), found 318.1185 (M^+).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C—H = 0.94–0.98 Å, N—H = 0.80 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(carrier).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{19}N_2S^+\cdot I^-$
M_r	446.33
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, b, c (Å)	8.6382 (3), 9.8182 (3), 12.1922 (4)
α, β, γ (°)	77.2839 (12), 85.1708 (11), 74.7224 (10)
V (Å^3)	972.66 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.76
Crystal size (mm)	0.27 × 0.21 × 0.15
Data collection	
Diffractometer	PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.649, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31969, 4853, 4594
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.063, 1.09
No. of reflections	4853
No. of parameters	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.43, −1.04

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXTL* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020).

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Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXTL* ((Sheldrick, 2008)).

N-[(Benzylsulfanyl)(phenylamino)methylidene]anilinium iodide

Crystal data

$C_{20}H_{19}N_2S^+\cdot I^-$
M_r = 446.33
Triclinic, $P\overline{1}$
a = 8.6382 (3) Å
b = 9.8182 (3) Å
c = 12.1922 (4) Å
α = 77.2839 (12)°
β = 85.1708 (11)°
γ = 74.7224 (10)°
V = 972.66 (6) Å^3
Z = 2
$F(000)$ = 444
D_x = 1.524 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9837 reflections
θ = 2.5–28.3°
μ = 1.76 mm^{-1}
T = 223 K
Block, colourless
0.27 × 0.21 × 0.15 mm

Data collection

PHOTON 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.649, T_{max} = 0.746
31969 measured reflections
4853 independent reflections
4594 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −11→11
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
S = 1.09
4853 reflections
225 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 0.8267P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.43 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.26986 (2)	0.34036 (2)	0.87755 (2)	0.04395 (6)
C1	0.3315 (2)	0.4161 (2)	0.28202 (17)	0.0316 (4)
C2	0.1753 (3)	0.4055 (3)	0.3116 (2)	0.0421 (5)
H2	0.1020	0.4181	0.2552	0.051*
C3	0.1274 (4)	0.3766 (3)	0.4237 (2)	0.0581 (7)
H3	0.0216	0.3697	0.4430	0.070*
C4	0.2340 (5)	0.3578 (3)	0.5072 (2)	0.0648 (8)
H4	0.2012	0.3380	0.5833	0.078*
C5	0.3880 (4)	0.3682 (3)	0.4786 (2)	0.0594 (7)
H5	0.4609	0.3550	0.5355	0.071*
C6	0.4373 (3)	0.3982 (2)	0.3666 (2)	0.0434 (5)
H6	0.5427	0.4064	0.3479	0.052*
C7	0.3883 (2)	0.4451 (2)	0.16100 (17)	0.0330 (4)
H7A	0.4058	0.3566	0.1320	0.040*
H7B	0.4917	0.4696	0.1574	0.040*
S1	0.24895 (6)	0.59022 (5)	0.07051 (4)	0.03231 (10)
C8	0.2092 (2)	0.72734 (19)	0.14740 (14)	0.0252 (3)
N1	0.32455 (19)	0.75297 (18)	0.19789 (14)	0.0278 (3)
H1N	0.415 (3)	0.724 (3)	0.177 (2)	0.036 (6)*
C9	0.3042 (2)	0.82793 (19)	0.28816 (15)	0.0267 (3)
C10	0.2028 (2)	0.7956 (2)	0.37864 (17)	0.0337 (4)
H10	0.1474	0.7243	0.3814	0.040*
C11	0.1841 (3)	0.8703 (3)	0.46533 (18)	0.0426 (5)
H11	0.1147	0.8502	0.5270	0.051*
C12	0.2668 (3)	0.9740 (3)	0.46136 (19)	0.0444 (5)
H12	0.2526	1.0250	0.5198	0.053*
C13	0.3700 (3)	1.0030 (2)	0.3723 (2)	0.0421 (5)
H13	0.4272	1.0727	0.3708	0.051*
C14	0.3903 (2)	0.9300 (2)	0.28442 (18)	0.0343 (4)
H14	0.4612	0.9493	0.2236	0.041*
N2	0.05644 (19)	0.80281 (17)	0.14673 (14)	0.0276 (3)
H2N	−0.010 (3)	0.765 (3)	0.134 (2)	0.034 (6)*
C15	−0.0057 (2)	0.94592 (19)	0.16504 (15)	0.0259 (3)
C16	0.0742 (2)	1.0527 (2)	0.12339 (16)	0.0310 (4)
H16	0.1723	1.0316	0.0832	0.037*
C17	0.0078 (3)	1.1909 (2)	0.14165 (18)	0.0380 (4)
H17	0.0622	1.2636	0.1148	0.046*
C18	−0.1379 (3)	1.2225 (2)	0.19912 (19)	0.0422 (5)
H18	−0.1816	1.3161	0.2122	0.051*

C19	−0.2187 (3)	1.1169 (2)	0.2371 (2)	0.0427 (5)
H19	−0.3192	1.1396	0.2743	0.051*
C20	−0.1536 (2)	0.9773 (2)	0.22119 (18)	0.0349 (4)
H20	−0.2086	0.9051	0.2479	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02782 (7)	0.04822 (9)	0.06798 (11)	−0.01720 (6)	0.01189 (6)	−0.03314 (7)
C1	0.0347 (10)	0.0226 (8)	0.0376 (10)	−0.0046 (7)	−0.0028 (8)	−0.0091 (7)
C2	0.0428 (12)	0.0421 (11)	0.0462 (12)	−0.0177 (9)	0.0024 (9)	−0.0122 (9)
C3	0.0661 (17)	0.0529 (15)	0.0582 (16)	−0.0274 (13)	0.0190 (13)	−0.0102 (12)
C4	0.099 (2)	0.0473 (15)	0.0396 (13)	−0.0139 (15)	0.0082 (14)	−0.0006 (11)
C5	0.079 (2)	0.0483 (14)	0.0424 (13)	0.0001 (13)	−0.0211 (13)	−0.0048 (11)
C6	0.0419 (12)	0.0377 (11)	0.0474 (12)	0.0001 (9)	−0.0127 (10)	−0.0102 (9)
C7	0.0294 (9)	0.0298 (9)	0.0393 (10)	−0.0018 (7)	−0.0002 (8)	−0.0136 (8)
S1	0.0365 (2)	0.0321 (2)	0.0301 (2)	−0.00373 (18)	−0.00340 (18)	−0.01509 (18)
C8	0.0254 (8)	0.0257 (8)	0.0253 (8)	−0.0059 (6)	0.0010 (6)	−0.0083 (6)
N1	0.0199 (7)	0.0326 (8)	0.0330 (8)	−0.0045 (6)	0.0014 (6)	−0.0146 (6)
C9	0.0231 (8)	0.0283 (8)	0.0294 (8)	−0.0030 (6)	−0.0050 (6)	−0.0104 (7)
C10	0.0331 (9)	0.0385 (10)	0.0329 (9)	−0.0115 (8)	−0.0011 (7)	−0.0117 (8)
C11	0.0459 (12)	0.0521 (13)	0.0331 (10)	−0.0119 (10)	0.0023 (9)	−0.0172 (9)
C12	0.0509 (13)	0.0452 (12)	0.0415 (11)	−0.0055 (10)	−0.0079 (10)	−0.0237 (10)
C13	0.0450 (12)	0.0372 (11)	0.0514 (13)	−0.0139 (9)	−0.0106 (10)	−0.0167 (9)
C14	0.0322 (9)	0.0348 (10)	0.0393 (10)	−0.0110 (8)	−0.0029 (8)	−0.0106 (8)
N2	0.0229 (7)	0.0292 (8)	0.0338 (8)	−0.0063 (6)	−0.0039 (6)	−0.0122 (6)
C15	0.0253 (8)	0.0262 (8)	0.0257 (8)	−0.0028 (6)	−0.0054 (6)	−0.0070 (6)
C16	0.0321 (9)	0.0324 (9)	0.0274 (8)	−0.0074 (7)	−0.0021 (7)	−0.0043 (7)
C17	0.0489 (12)	0.0300 (9)	0.0353 (10)	−0.0118 (9)	−0.0066 (9)	−0.0025 (8)
C18	0.0523 (13)	0.0287 (10)	0.0416 (11)	0.0008 (9)	−0.0057 (9)	−0.0108 (8)
C19	0.0368 (11)	0.0405 (11)	0.0460 (12)	0.0010 (9)	0.0052 (9)	−0.0143 (9)
C20	0.0300 (9)	0.0342 (10)	0.0406 (10)	−0.0071 (8)	0.0024 (8)	−0.0105 (8)

Geometric parameters (Å, º)

C1—C6	1.386 (3)	C10—C11	1.390 (3)
C1—C2	1.392 (3)	C10—H10	0.9400
C1—C7	1.505 (3)	C11—C12	1.381 (3)
C2—C3	1.383 (4)	C11—H11	0.9400
C2—H2	0.9400	C12—C13	1.374 (4)
C3—C4	1.381 (5)	C12—H12	0.9400
C3—H3	0.9400	C13—C14	1.391 (3)
C4—C5	1.371 (5)	C13—H13	0.9400
C4—H4	0.9400	C14—H14	0.9400
C5—C6	1.388 (4)	N2—C15	1.426 (2)
C5—H5	0.9400	N2—H2N	0.81 (3)
C6—H6	0.9400	C15—C16	1.386 (3)
C7—S1	1.823 (2)	C15—C20	1.391 (3)

C7—H7A	0.9800	C16—C17	1.386 (3)
C7—H7B	0.9800	C16—H16	0.9400
S1—C8	1.7513 (18)	C17—C18	1.383 (3)
C8—N1	1.319 (2)	C17—H17	0.9400
C8—N2	1.332 (2)	C18—C19	1.376 (4)
N1—C9	1.428 (2)	C18—H18	0.9400
N1—H1N	0.80 (3)	C19—C20	1.388 (3)
C9—C10	1.384 (3)	C19—H19	0.9400
C9—C14	1.388 (3)	C20—H20	0.9400

C6—C1—C2	118.9 (2)	C9—C10—H10	120.5
C6—C1—C7	119.46 (19)	C11—C10—H10	120.5
C2—C1—C7	121.67 (19)	C12—C11—C10	120.3 (2)
C3—C2—C1	120.3 (2)	C12—C11—H11	119.9
C3—C2—H2	119.8	C10—C11—H11	119.9
C1—C2—H2	119.8	C13—C12—C11	120.3 (2)
C4—C3—C2	120.4 (3)	C13—C12—H12	119.9
C4—C3—H3	119.8	C11—C12—H12	119.9
C2—C3—H3	119.8	C12—C13—C14	120.5 (2)
C5—C4—C3	119.6 (3)	C12—C13—H13	119.8
C5—C4—H4	120.2	C14—C13—H13	119.8
C3—C4—H4	120.2	C9—C14—C13	118.8 (2)
C4—C5—C6	120.6 (3)	C9—C14—H14	120.6
C4—C5—H5	119.7	C13—C14—H14	120.6
C6—C5—H5	119.7	C8—N2—C15	127.80 (16)
C1—C6—C5	120.2 (2)	C8—N2—H2N	117.4 (18)
C1—C6—H6	119.9	C15—N2—H2N	114.8 (18)
C5—C6—H6	119.9	C16—C15—C20	120.73 (17)
C1—C7—S1	113.83 (13)	C16—C15—N2	121.30 (17)
C1—C7—H7A	108.8	C20—C15—N2	117.89 (17)
S1—C7—H7A	108.8	C17—C16—C15	119.28 (19)
C1—C7—H7B	108.8	C17—C16—H16	120.4
S1—C7—H7B	108.8	C15—C16—H16	120.4
H7A—C7—H7B	107.7	C18—C17—C16	120.3 (2)
C8—S1—C7	101.66 (9)	C18—C17—H17	119.8
N1—C8—N2	124.53 (16)	C16—C17—H17	119.8
N1—C8—S1	121.30 (14)	C19—C18—C17	120.0 (2)
N2—C8—S1	114.14 (13)	C19—C18—H18	120.0
C8—N1—C9	126.22 (16)	C17—C18—H18	120.0
C8—N1—H1N	118.0 (19)	C18—C19—C20	120.7 (2)
C9—N1—H1N	115.7 (19)	C18—C19—H19	119.7
C10—C9—C14	121.18 (18)	C20—C19—H19	119.7
C10—C9—N1	119.87 (17)	C19—C20—C15	118.9 (2)
C14—C9—N1	118.93 (17)	C19—C20—H20	120.5
C9—C10—C11	119.0 (2)	C15—C20—H20	120.5

C6—C1—C2—C3	−0.5 (3)	C9—C10—C11—C12	−0.6 (3)
C7—C1—C2—C3	179.0 (2)	C10—C11—C12—C13	−0.8 (4)

C1—C2—C3—C4	0.0 (4)	C11—C12—C13—C14	1.0 (4)
C2—C3—C4—C5	0.1 (4)	C10—C9—C14—C13	−1.7 (3)
C3—C4—C5—C6	0.3 (4)	N1—C9—C14—C13	179.86 (18)
C2—C1—C6—C5	0.9 (3)	C12—C13—C14—C9	0.3 (3)
C7—C1—C6—C5	−178.6 (2)	N1—C8—N2—C15	21.8 (3)
C4—C5—C6—C1	−0.8 (4)	S1—C8—N2—C15	−156.34 (15)
C6—C1—C7—S1	−134.43 (17)	C8—N2—C15—C16	38.5 (3)
C2—C1—C7—S1	46.1 (2)	C8—N2—C15—C20	−144.78 (19)
C1—C7—S1—C8	49.53 (16)	C20—C15—C16—C17	2.2 (3)
C7—S1—C8—N1	41.74 (18)	N2—C15—C16—C17	178.92 (17)
C7—S1—C8—N2	−140.01 (15)	C15—C16—C17—C18	−1.1 (3)
N2—C8—N1—C9	22.1 (3)	C16—C17—C18—C19	−0.9 (3)
S1—C8—N1—C9	−159.85 (15)	C17—C18—C19—C20	1.8 (4)
C8—N1—C9—C10	46.0 (3)	C18—C19—C20—C15	−0.7 (3)
C8—N1—C9—C14	−135.6 (2)	C16—C15—C20—C19	−1.4 (3)
C14—C9—C10—C11	1.9 (3)	N2—C15—C20—C19	−178.16 (18)
N1—C9—C10—C11	−179.70 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···I1^{i}	0.80 (3)	2.69 (3)	3.4781 (17)	171 (2)
N2—H2*N*···I1^{ii}	0.80 (3)	2.73 (3)	3.5242 (17)	169 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1.