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

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In the title molecular salt, C_{20}H_{19}N_{2}S^{+}/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_{2})_{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_{2}S^{+}−I^{-} are reported herein.

2. Structural commentary

The title compound, C_{20}H_{19}N_{2}S^{+}−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
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 [\(\text{C1—C7—S1—C8} = 49.53 (16)°\)]. 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] (\(\text{Ar} = 1,4\)-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 \(\pi\)-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

|          | \(D—\cdot—H—\cdot—A\) | \(D—H\) | \(H—\cdot—A\) | \(D—\cdot—H\) |
|----------|------------------------|---------|---------------|--------------|
| N1—H11N—\cdot—H1' | 0.80 (3) | 2.69 (3) | 3.4781 (17) | 171 (2) |
| N2—H2N—\cdot—H2a | 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 \(N—H—\cdot—I\) 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 \(\pi—\pi\) 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...
the title compound are the range 102.6 to 104.8°, depending on the counter-ions (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 a 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;1H NMR (300 MHz, DMSO): δ 7.21–7.39 (m, 15 H), δ 4.45 (s, 2 H); HR TOF–MS for C20H18N2S+: calculated 318.1186, found 318.1185 (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 . 8 0 Å) and refined using a riding model withUiso(H) = 1.2Ueq(carrier).

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Table 2

| Table 2 | Experimental details. |
|---------|-----------------------|
| Crystal data | C20H18N2S+: calculated 318.1186, found 318.1185 (M+) |
| Chemical formula | C20H18N2S+ |
| Mw | 446.33 |
| Crystal system, space group | Triclinic, Pτ |
| 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 (Å³) | 972.66 (6) |
| Z | 2 |
| Radiation type | Mo Kα |
| μ (mm⁻¹) | 1.76 |
| Crystal size (mm) | 0.27 × 0.21 × 0.15 |
| Data collection | PHOTON 100 CMOS |
| Diffractometer | Multi-scan (SADABS; Bruker, 2016) |
| Absorption correction | Reflections |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 0.023 |
| Rint | 0.025, 0.063, 1.09 |
| No. of reflections | 4853 |
| No. of parameters | 225 |
| H-atoms treatment | H atoms treated by a mixture of independent and constrained refinement |
| Δρmax, Δρmin (e Å⁻³) | 1.43, −1.04 |

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

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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
\[\text{C}_{20}\text{H}_{19}\text{N}_{2}\text{S}^{+}\cdot\text{I}^{-}\]
\[M_r = 446.33\]
Triclinic, \(P\bar{1}\)
\(a = 8.6382\) (3) Å
\(b = 9.8182\) (3) Å
\(c = 12.1922\) (4) Å
\(\alpha = 77.2839\) (12)°
\(\beta = 85.1708\) (11)°
\(\gamma = 74.7224\) (10)°
\(V = 972.66\) (6) Å³

\(Z = 2\)
\(F(000) = 444\)
\(D_x = 1.524\) Mg m⁻³
Mo Kα radiation, \(\lambda = 0.71073\) Å
Cell parameters from 9837 reflections
\(\theta = 2.5–28.3°\)
\(\mu = 1.76\) mm⁻¹
\(T = 223\) K
Block, colourless
0.27 × 0.21 × 0.15 mm

Data collection
PHOTON 100 CMOS diffractometer
\(\varphi\) and \(\omega\) scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
\(T_{\text{min}} = 0.649, T_{\text{max}} = 0.746\)
31969 measured reflections
4853 independent reflections
4594 reflections with \(|I| > 2\sigma(I)\)
\(R_{\text{int}} = 0.023\)
\(\theta_{\text{max}} = 28.3°, \theta_{\text{min}} = 2.2°\)
\(h = -11\rightarrow 11\)
\(k = -13\rightarrow 13\)
\(l = -16\rightarrow 16\)

Refinement
Refinement on \(F^2\)
Least-squares matrix: full
\(R[F^2 > 2\sigma(F^2)] = 0.025\)
\(wR(F^2) = 0.063\)
\(S = 1.09\)
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
\(w = 1/[\sigma(F_c^2) + (0.0253P)^2 + 0.8267P]\)
where \(P = (F_c^2 + 2F_s^2)/3\)
\((\Delta\sigma)_{\text{max}} = 0.001\)
\(\Delta\rho_{\text{max}} = 1.43\) e Å⁻³
\(\Delta\rho_{\text{min}} = -1.03\) 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          | Ueq/Isu* |
|---|------------|------------|------------|----------|
| 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)**

|     | U¹¹   | U¹²   | U¹³   | U²²   | U²³   | U³³   |
|-----|-------|-------|-------|-------|-------|-------|
| 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) | 0.0009 (11) | -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, °)**

|     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 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  C13—C14—C13  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—H1N···I1i | 0.80 (3) | 2.69 (3) | 3.4781 (17) | 171 (2) |
| N2—H2N···I1ii | 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.