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# 3,5-Diphenyl-1,2,4-dithiazolium tetrabromidoferrate(III)

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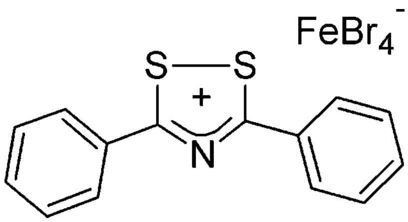
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.027; $wR$ factor = 0.050; data-to-parameter ratio = 22.2.

The cation of the title salt, $(C_{14}H_{10}NS_2)[FeBr_4]$, contains a flat central $NC_2S_2$ ring (r.m.s. deviation = 0.005 Å), with two attached phenyl rings that are almost coplanar [the dihedral angles between the mean planes are 2.4 (1) and 7.7 (1)° for the two phenyl rings]. The $[FeBr_4]^-$ anion makes short Br···S contacts [Br···S = 3.4819 (8), 3.6327 (9) and 3.5925 (9) Å] and also bridges by way of short contacts to ring H atoms of a second cation held parallel to the first by $\pi$-stacking, with a separation between the mean 1,2,4-dithiazolium rings of 3.409 Å. The closest contacts are between a phenyl ring centroid of one cation and the *ipso* C atom of the phenyl ring of another cation, for which the distance is 3.489 Å. The discrete dimers are linked laterally by further Br···H short contacts, resulting in double sheets located parallel to the $b$ axis and to the bisector of $a$ and $c$.

## Related literature

For synthesis details, see: Corsaro *et al.* (1984); Liebscher & Hartmann (1977). For related structures, see: Clegg *et al.* (1996); Neels *et al.* (1986). For a description of the Cambridge Structural Database, see: Allen (2002). For bond lengths in tetrabromidoferrate complexes, see: Maithufi & Otto (2011); Bhattacharya & Sarkar (2010). For short-contact distances between stacked aryl rings, see: Martinez & Iverson (2012); McGaughey *et al.* (1998).



## Experimental

### Crystal data

| | |
|---|---|
| $(C_{14}H_{10}NS_2)[FeBr_4]$ | $V$ = 1906.51 (17) Å$^3$ |
| $M_r$ = 631.84 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 10.6492 (5) Å | $\mu$ = 9.39 mm$^{-1}$ |
| $b$ = 11.4005 (6) Å | $T$ = 173 K |
| $c$ = 15.8046 (8) Å | 0.22 × 0.13 × 0.07 mm |
| $\beta$ = 96.482 (1)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 27655 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | 4426 independent reflections |
| $T_{min}$ = 0.556, $T_{max}$ = 0.746 | 3497 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.042 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.027 | 199 parameters |
| $wR(F^2)$ = 0.050 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 0.63 e Å$^{-3}$ |
| 4426 reflections | $\Delta\rho_{min}$ = −0.45 e Å$^{-3}$ |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The Natural Sciences and Engineering Research Council of Canada (NSERC) is gratefully acknowledged for a Discovery Grant. The diffractometer was purchased with the help of NSERC and the University of Lethbridge.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2091).

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# supporting information

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## 3,5-Diphenyl-1,2,4-dithiazolium tetrabromidoferrate(III)

**Ibukun O. Shotonwa and René T. Boeré**

### S1. Comment

The structure of a cation–anion pair in (I) as found in the crystal lattice is shown in Fig. 1, wherein the short contacts from the anion Br atoms to the S atoms of the cation are highlighted. An extended diagram showing the dimerization of two rings through short inter-ring interactions and their lateral extensions into planes *via* short contacts between ring S and H atoms with the $[FeBr_4]^-$ anions is shown in Fig. 2. The separation between the approximately planar dimer components of 3.409 Å corresponds to typical minimum distances for off-center parallel stacking of electron-rich aromatic rings (Martinez & Iverson, 2012; McGaughey *et al.*, 1998).

Only two previous structures (II) and (III) are reported in the literature for 3,5-diaryl-1,2,4-dithiazolium ring compounds. For (II), the same 3,5-diphenyl-1,2,4-dithiazolium cation crystallizes with a large azathiophosphine cage anion, 1,3,5,7-tetrathioxo-10-aza-2,4,6,8,9-pentathia-1$\lambda^5$,3$\lambda^5$,5$\lambda^5$,7$\lambda^5$-tetraphosphatricyclo(3.3.1.1$^{3,7}$)decanide [Cambridge Structural Database (Allen, 2002) refcode FARXIF (Neels *et al.*, 1986)]. For (III), the anion is the more conventional $AsF_6^-$, but the substituents are 2-methylbenzene rings [refcode TEHRED (Clegg *et al.*, 1996)]. The S—S bond in (I) at 2.019 (1) Å is significantly longer than that in (III) at 2.004 (1) Å, but is within the e.s.d. range of that found in (II) at 2.008 (5) Å. A possible reason for the longer bond in (I) is the presence of stronger sulfur-halogen non-bonded contact interactions than occur for $AsF_6^-$. The packing arrangements in (II) and (III) do not involve cation ring dimerization as observed in (I).

The bond distances in the $[FeBr_4]^-$ anion are entirely normal for high spin Fe$^{III}$ (Fe—Br (av) = 2.332 (3) Å). For example, in a recent structure by Bhattacharya & Sarkar (2010) [refcode AKAZOC], Fe—Br (av) = 2.332 (7) Å. Distances in $FeBr_4^{2-}$ (*i.e.* an Fe$^{II}$ anion) are as much as 6% longer (Maithufi & Otto, 2011).

### S2. Experimental

Crystals of (I) were obtained as a minor component during the synthesis of 3,5-diphenyl-1,2,4-dithiazolium perchlorate from *N,N*-dimorpholino-thiobenzamide bromine adduct and unsubstituted thiobenzamide in chloroform using the method of Corsaro *et al.* (1984). The intermediates are taken up in 6 N $HClO_4$ which is supposed to afford the perchlorate salt of the dithiazolium (Liebscher & Hartmann, 1977). The source of the iron is presumed to be rust that was digested by the perchloric acid, because the ferric aqua ion would be ripe for ligation by strongly nucleophilic bromide ions present as a byproduct from the previous step. Crystals of (I) form as well shaped red–orange prisms amongst the thin yellow plates of perchlorate salt, m.p. 169.3–171.1°C.

### S3. Refinement

All H atoms were located on a difference map, but for purposes of refinement are treated as riding on their attached aromatic C atoms with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

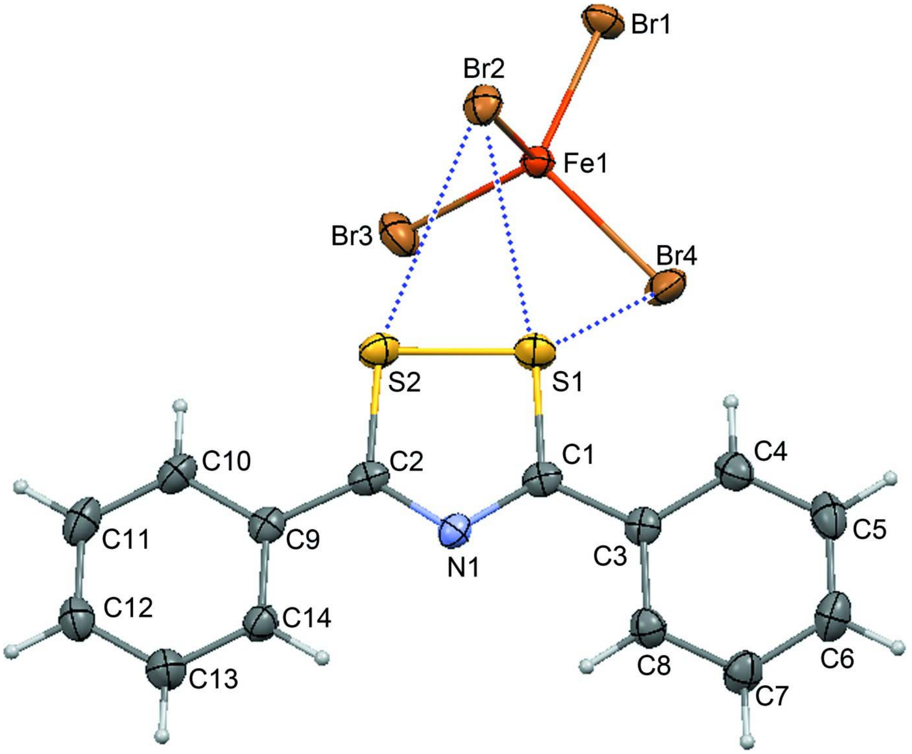

**Figure 1**

A view of (I) plotted with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as spheres of arbitrary radius. Dotted lines indicate the short cation–anion contacts Br2···S1 = 3.4819 (8), Br2···S2 = 3.6327 (9) and Br4···S1 = 3.5925 (9) Å.

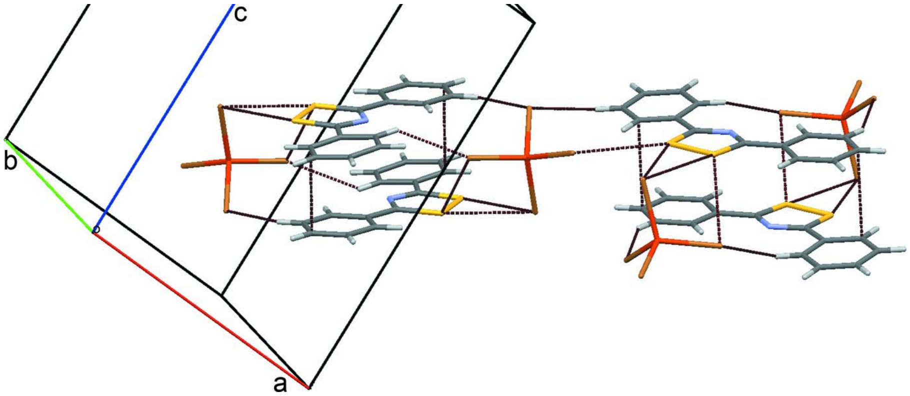

**Figure 2**

Short off-center parallel stacking of electron-rich aromatic rings leads to sheets of double layers parallel to *b* and bisecting the *a* and *c* axes; $[FeBr_4]^-$ anions bridge between the upper and lower double-layer components.

### 3,5-Diphenyl-1,2,4-dithiazolium tetrabromidoferrate(III)

*Crystal data*

| | |
|---|---|
| $(C_{14}H_{10}NS_2)[FeBr_4]$ | Hall symbol: -P 2ybc |
| $M_r$ = 631.84 | $a$ = 10.6492 (5) Å |
| Monoclinic, $P2_1/c$ | $b$ = 11.4005 (6) Å |

$c = 15.8046$ (8) Å
$\beta = 96.482$ (1)°
$V = 1906.51$ (17) Å$^3$
$Z = 4$
$F(000) = 1196$
Standard setting
$D_x = 2.201$ Mg m$^{-3}$
Melting point: 442.5 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9924 reflections
$\theta = 2.2$–27.5°
$\mu = 9.39$ mm$^{-1}$
$T = 173$ K
Prism, red
0.22 × 0.13 × 0.07 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube, Bruker D8
Graphite monochromator
Detector resolution: 66.06 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)

$T_{\min} = 0.556$, $T_{\max} = 0.746$
27655 measured reflections
4426 independent reflections
3497 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$
$\theta_{\max} = 27.7°$, $\theta_{\min} = 1.9°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -20 \rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.050$
$S = 1.02$
4426 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 0.6153P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.63$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.45$ e Å$^{-3}$

*Special details*

**Experimental**. A crystal coated in Paratone (TM) oil was mounted on the end of a thin glass capillary and cooled in the gas stream of the diffractometer Kryoflex device.

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

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

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

| | $x$ | $y$ | $z$ | $U_{\rm iso}$*/$U_{\rm eq}$ |
|---|---|---|---|---|
| Br2 | 0.52392 (3) | 0.78560 (3) | 0.368206 (19) | 0.03449 (8) |
| S2 | 0.66283 (7) | 0.51567 (7) | 0.45795 (5) | 0.03375 (18) |
| S1 | 0.76220 (7) | 0.65596 (7) | 0.50609 (5) | 0.03592 (18) |
| N1 | 0.8648 (2) | 0.4568 (2) | 0.56025 (14) | 0.0258 (5) |
| C1 | 0.8760 (2) | 0.5727 (2) | 0.56450 (16) | 0.0264 (6) |
| C2 | 0.7649 (3) | 0.4159 (3) | 0.51171 (16) | 0.0273 (6) |
| C3 | 0.9797 (3) | 0.6304 (2) | 0.61626 (17) | 0.0266 (6) |

| | | | | |
|---|---|---|---|---|
| C4 | 0.9917 (3) | 0.7527 (3) | 0.61675 (19) | 0.0342 (7) |
| H4 | 0.9323 | 0.7991 | 0.5821 | 0.041* |
| C5 | 1.0893 (3) | 0.8059 (3) | 0.6672 (2) | 0.0412 (8) |
| H5 | 1.0965 | 0.8889 | 0.6681 | 0.049* |
| C6 | 1.1764 (3) | 0.7384 (3) | 0.71628 (19) | 0.0399 (8) |
| H6 | 1.2439 | 0.7751 | 0.7509 | 0.048* |
| C7 | 1.1665 (3) | 0.6175 (3) | 0.71570 (18) | 0.0371 (7) |
| H7 | 1.2274 | 0.5717 | 0.7497 | 0.045* |
| C8 | 1.0687 (3) | 0.5628 (3) | 0.66606 (17) | 0.0315 (7) |
| H8 | 1.0621 | 0.4797 | 0.6658 | 0.038* |
| C9 | 0.7397 (3) | 0.2903 (2) | 0.50317 (17) | 0.0276 (6) |
| C10 | 0.6429 (3) | 0.2465 (3) | 0.44497 (18) | 0.0347 (7) |
| H10 | 0.5910 | 0.2985 | 0.4094 | 0.042* |
| C11 | 0.6230 (3) | 0.1269 (3) | 0.4395 (2) | 0.0416 (8) |
| H11 | 0.5574 | 0.0966 | 0.3998 | 0.050* |
| C12 | 0.6980 (3) | 0.0510 (3) | 0.49137 (18) | 0.0369 (7) |
| H12 | 0.6839 | −0.0312 | 0.4871 | 0.044* |
| C13 | 0.7932 (3) | 0.0946 (3) | 0.5493 (2) | 0.0379 (7) |
| H13 | 0.8441 | 0.0423 | 0.5853 | 0.045* |
| C14 | 0.8147 (3) | 0.2137 (2) | 0.55519 (18) | 0.0311 (7) |
| H14 | 0.8808 | 0.2434 | 0.5948 | 0.037* |
| Fe1 | 0.67510 (4) | 0.82072 (3) | 0.27504 (2) | 0.02488 (10) |
| Br1 | 0.61558 (3) | 0.98672 (3) | 0.194423 (18) | 0.03480 (8) |
| Br3 | 0.68944 (3) | 0.65879 (3) | 0.18652 (2) | 0.04436 (9) |
| Br4 | 0.87224 (3) | 0.85136 (3) | 0.35206 (2) | 0.04081 (9) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br2 | 0.02809 (16) | 0.03810 (18) | 0.03845 (17) | −0.00452 (13) | 0.00891 (13) | 0.00027 (13) |
| S2 | 0.0321 (4) | 0.0389 (4) | 0.0287 (4) | 0.0031 (3) | −0.0038 (3) | 0.0027 (3) |
| S1 | 0.0400 (4) | 0.0333 (4) | 0.0329 (4) | 0.0022 (3) | −0.0029 (3) | 0.0078 (3) |
| N1 | 0.0239 (12) | 0.0289 (13) | 0.0247 (12) | −0.0012 (10) | 0.0031 (10) | −0.0007 (10) |
| C1 | 0.0246 (15) | 0.0331 (17) | 0.0227 (14) | 0.0011 (12) | 0.0078 (12) | 0.0033 (12) |
| C2 | 0.0241 (15) | 0.0370 (17) | 0.0214 (14) | 0.0034 (12) | 0.0046 (12) | 0.0039 (12) |
| C3 | 0.0276 (15) | 0.0306 (16) | 0.0228 (14) | −0.0027 (12) | 0.0089 (12) | 0.0015 (12) |
| C4 | 0.0327 (17) | 0.0301 (17) | 0.0413 (18) | 0.0011 (13) | 0.0104 (14) | 0.0039 (14) |
| C5 | 0.0426 (19) | 0.0318 (18) | 0.051 (2) | −0.0102 (15) | 0.0146 (16) | −0.0056 (15) |
| C6 | 0.0397 (19) | 0.046 (2) | 0.0337 (17) | −0.0143 (15) | 0.0019 (14) | −0.0044 (15) |
| C7 | 0.0392 (18) | 0.0401 (19) | 0.0307 (17) | −0.0056 (14) | −0.0019 (14) | 0.0038 (14) |
| C8 | 0.0362 (17) | 0.0290 (16) | 0.0294 (16) | −0.0023 (13) | 0.0044 (13) | 0.0021 (13) |
| C9 | 0.0258 (15) | 0.0332 (16) | 0.0246 (14) | −0.0017 (12) | 0.0065 (12) | −0.0014 (12) |
| C10 | 0.0273 (16) | 0.045 (2) | 0.0303 (16) | −0.0031 (14) | −0.0017 (13) | −0.0023 (14) |
| C11 | 0.0351 (18) | 0.053 (2) | 0.0358 (18) | −0.0111 (16) | 0.0003 (14) | −0.0103 (16) |
| C12 | 0.0405 (19) | 0.0312 (17) | 0.0397 (18) | −0.0052 (14) | 0.0078 (15) | −0.0068 (14) |
| C13 | 0.0378 (18) | 0.0344 (18) | 0.0409 (18) | −0.0014 (14) | 0.0019 (14) | −0.0007 (14) |
| C14 | 0.0286 (16) | 0.0334 (17) | 0.0303 (15) | −0.0026 (13) | −0.0010 (12) | −0.0026 (13) |
| Fe1 | 0.0231 (2) | 0.0242 (2) | 0.0271 (2) | 0.00182 (16) | 0.00160 (16) | 0.00272 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Br1 | 0.04259 (18) | 0.02889 (16) | 0.03186 (16) | 0.00849 (13) | −0.00040 (13) | 0.00606 (12) |
| Br3 | 0.0519 (2) | 0.02974 (18) | 0.0529 (2) | 0.00340 (15) | 0.01216 (16) | −0.00932 (15) |
| Br4 | 0.02328 (15) | 0.0481 (2) | 0.0491 (2) | −0.00342 (14) | −0.00431 (13) | 0.01204 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br2—Fe1 | 2.3357 (5) | C7—H7 | 0.9500 |
| S2—C2 | 1.729 (3) | C8—H8 | 0.9500 |
| S2—S1 | 2.0186 (11) | C9—C14 | 1.389 (4) |
| S1—C1 | 1.723 (3) | C9—C10 | 1.394 (4) |
| N1—C2 | 1.324 (3) | C10—C11 | 1.381 (4) |
| N1—C1 | 1.329 (3) | C10—H10 | 0.9500 |
| C1—C3 | 1.455 (4) | C11—C12 | 1.382 (4) |
| C2—C9 | 1.460 (4) | C11—H11 | 0.9500 |
| C3—C8 | 1.394 (4) | C12—C13 | 1.379 (4) |
| C3—C4 | 1.399 (4) | C12—H12 | 0.9500 |
| C4—C5 | 1.377 (4) | C13—C14 | 1.379 (4) |
| C4—H4 | 0.9500 | C13—H13 | 0.9500 |
| C5—C6 | 1.375 (4) | C14—H14 | 0.9500 |
| C5—H5 | 0.9500 | Fe1—Br1 | 2.3291 (5) |
| C6—C7 | 1.382 (4) | Fe1—Br4 | 2.3311 (5) |
| C6—H6 | 0.9500 | Fe1—Br3 | 2.3317 (5) |
| C7—C8 | 1.380 (4) | | |

| | | | |
|---|---|---|---|
| C2—S2—S1 | 93.58 (10) | C3—C8—H8 | 120.2 |
| C1—S1—S2 | 94.17 (10) | C14—C9—C10 | 119.9 (3) |
| C2—N1—C1 | 116.2 (2) | C14—C9—C2 | 118.3 (2) |
| N1—C1—C3 | 122.4 (2) | C10—C9—C2 | 121.8 (3) |
| N1—C1—S1 | 117.9 (2) | C11—C10—C9 | 119.4 (3) |
| C3—C1—S1 | 119.7 (2) | C11—C10—H10 | 120.3 |
| N1—C2—C9 | 121.8 (2) | C9—C10—H10 | 120.3 |
| N1—C2—S2 | 118.2 (2) | C10—C11—C12 | 120.5 (3) |
| C9—C2—S2 | 120.1 (2) | C10—C11—H11 | 119.8 |
| C8—C3—C4 | 119.5 (3) | C12—C11—H11 | 119.8 |
| C8—C3—C1 | 119.5 (3) | C13—C12—C11 | 120.0 (3) |
| C4—C3—C1 | 121.1 (3) | C13—C12—H12 | 120.0 |
| C5—C4—C3 | 120.3 (3) | C11—C12—H12 | 120.0 |
| C5—C4—H4 | 119.9 | C14—C13—C12 | 120.3 (3) |
| C3—C4—H4 | 119.9 | C14—C13—H13 | 119.9 |
| C6—C5—C4 | 119.8 (3) | C12—C13—H13 | 119.9 |
| C6—C5—H5 | 120.1 | C13—C14—C9 | 119.9 (3) |
| C4—C5—H5 | 120.1 | C13—C14—H14 | 120.0 |
| C5—C6—C7 | 120.5 (3) | C9—C14—H14 | 120.0 |
| C5—C6—H6 | 119.7 | Br1—Fe1—Br4 | 109.714 (19) |
| C7—C6—H6 | 119.7 | Br1—Fe1—Br3 | 110.324 (19) |
| C8—C7—C6 | 120.4 (3) | Br4—Fe1—Br3 | 108.411 (19) |
| C8—C7—H7 | 119.8 | Br1—Fe1—Br2 | 108.648 (19) |
| C6—C7—H7 | 119.8 | Br4—Fe1—Br2 | 109.921 (19) |

| | | | |
|---|---|---|---|
| C7—C8—C3 | 119.5 (3) | Br3—Fe1—Br2 | 109.817 (19) |
| C7—C8—H8 | 120.2 | | |