Crystal structures of trans-dichloridotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II), trans-dibromidotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II) and trans-dibromidotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II) diethyl ether disolvate

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The title compounds, [FeCl₂(C₁₅H₁₄N₂)₄], (I), [FeBr₂(C₁₅H₁₂N₂)₄], (II), and [FeBr₂(C₁₅H₁₂N₂)₄]-2C₂H₅O, (IIb), respectively, all have triclinic symmetry, with (I) and (II) being isotypic. The Fe⁺⁺ atoms in each of the structures are located on an inversion center. They have octahedral FeX₄ (X = Cl and Br, respectively) coordination spheres with the Fe⁺⁺ atom coordinated by two halide ions in a trans arrangement and by the tertiary N atom of four arylimidazole ligands [1-(2,6-diisopropylphenyl)-1H-imidazole] in the equatorial plane. In the two independent ligands, the benzene and imidazole rings are almost normal to one another, with dihedral angles of 88.19 (15) and 79.26 (14)° in (I), 87.0 (3) and 79.2 (3)° in (II), and 84.71 (11) and 80.58 (13)° in (IIb). The imidazole rings of the two independent ligand molecules are inclined to one another by 70.04 (15), 69.3 (3) and 61.55 (12)°, respectively, while the benzene rings are inclined to one another by 82.83 (13), 83.0 (2) and 88.16 (12)°, respectively. The various dihedral angles involving (IIb) differ slightly from those in (I) and (II), probably due to the close proximity of the diethyl ether solvent molecule. There are a number of C—H···halide hydrogen bonds in each molecule involving the CH groups of the imidazole units. In the structures of compounds (I) and (II), molecules are linked via pairs of C—H···halogen hydrogen bonds, forming chains along the a axis that enclose R₂(12) ring motifs. The chains are linked by C—H···π interactions, forming sheets parallel to (001). In the structure of compound (IIb), molecules are linked via pairs of C—H···halogen hydrogen bonds, forming chains along the b axis, and the diethyl ether solvent molecules are attached to the chains via C—H···O hydrogen bonds. The chains are linked by C—H···π interactions, forming sheets parallel to (001). In (I) and (II), the methyl groups of an isopropyl group are disordered over two positions [occupancy ratio = 0.727 (13):0.273 (13) and 0.5:0.5, respectively]. In (IIb), one of the ethyl groups of the diethyl ether solvent molecule is disordered over two positions (occupancy ratio = 0.5:0.5).

1. Chemical context

The use of organometallic complexes as catalysts is an important development in the field of material chemistry. However, despite this, only a very few of them contain iron(II), except the tridentate diimine pyridine complex (Small et al., 1998; Small & Brookhart, 1998; Britovsek et al., 1998) used in olefin polymerization. Unfortunately, this model
suffers from its lack of tolerance towards the minor changes carried out in its envelope, resulting in a drastic reduction of its catalytic activity. Neutral and cationic complexes of iron(II) chloride and bromide with nitrogen bases are well known for imidazole, pyridine and pyrazoles (Schröder et al., 2009; Christie et al., 1993). For this reason, we set out to prepare new iron complexes containing more electron-donating and bulky ligands. Only a few analogous bulky arylimidazoles have been reported so far (Reisner et al., 2007).

We focused our attention on the use of bis-N-heterocyclic carbene Fe^{II} complexes in hydrogenation and polymerization of olefins (Mafua, 2006). During the preparation of these complexes, several other complexes of Fe^{II} and Fe^{III} were isolated, among them the title compounds, (I), (II) and (IIb). Compound (I) was isolated by deprotonation of bis-imidazoliummethylene tetrachloridoferrate(III) (L1 in Fig. 7) with NaH in THF at reflux. When the same reaction was conducted at room temperature, only the starting material was recovered after recrystallization. Compounds (II) and (IIb) were isolated when bisimidazoliummethylene tetrabromido-ferrate(III) (L2 in Fig. 7) was reacted with NaH in THF at reflux. The main result in the structure of these compounds is the loss of the bridging methylene group of the starting bisimidazolium cation. Thus two independent N-1-arylimidazolyl groups are formed for each starting bisimidazolium cation. Additionally, this result demonstrates a possible fragility of methylene-bisimidazole ligands when used in harsh reaction conditions. The question of the reduction of Fe^{III} to Fe^{II} remains to be elucidated.

2. Structural commentary

The structures of (I) and (II) are isotypic whereas (IIb) differs due to the presence of solvent diethyl ether molecules. The whole molecule of each compound, (I), (II) and (IIb), is generated by inversion symmetry (Figs. 1, 2 and 3, respectively). The Fe^{II} atom, Fe1, is located on an inversion center.
Table 1
Hydrogen-bond geometry (Å, °) for (I).

| D—H···A | D—H | H···A | D····A | D—H···A |
|---------|------|-------|--------|--------|
| C1—H1—Cl1 | 0.95 | 2.62 | 3.257 (3) | 125 |
| C2—H2—Cl1 | 0.95 | 2.92 | 3.433 (3) | 115 |
| C16—H16—Cl1 | 0.95 | 2.76 | 3.294 (3) | 117 |
| C17—H17—Cl1 | 0.95 | 2.82 | 3.375 (3) | 118 |
| C18—H18—Cl1 | 0.95 | 2.70 | 3.629 (3) | 166 |
| C27—H27A—Cg3m | 0.98 | 2.79 | 3.562 (4) | 136 |
| C30—H30C—Cg3m | 0.98 | 2.92 | 3.901 (4) | 176 |

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

| D—H···A | D—H | H···A | D····A | D—H···A |
|---------|------|-------|--------|--------|
| C1—H1—Br1 | 0.95 | 2.71 | 3.368 (4) | 127 |
| C2—H2—Br1 | 0.95 | 2.91 | 3.477 (5) | 119 |
| C16—H16—Br1 | 0.95 | 2.81 | 3.373 (4) | 119 |
| C17—H17—Br1 | 0.95 | 2.91 | 3.484 (4) | 120 |
| C18—H18—Br1 | 0.95 | 2.77 | 3.707 (5) | 167 |
| C27—H27A—Cg4m | 0.98 | 2.92 | 3.639 (6) | 131 |
| C30—H30C—Cg3m | 0.98 | 2.88 | 3.862 (6) | 177 |

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

Table 3
Hydrogen-bond geometry (Å, °) for (IIb).

| D—H···A | D—H | H···A | D····A | D—H···A |
|---------|------|-------|--------|--------|
| C1—H1—Br1 | 0.95 | 2.76 | 3.399 (2) | 125 |
| C2—H2—Br1 | 0.95 | 2.89 | 3.479 (2) | 121 |
| C16—H16—Br1 | 0.95 | 2.86 | 3.4119 (18) | 118 |
| C17—H17—Br1 | 0.95 | 3.02 | 3.542 (2) | 116 |
| C18—H18—O1m | 0.95 | 2.40 | 3.337 (3) | 170 |
| C15—H15A—Cg3m | 0.98 | 2.92 | 3.801 (3) | 150 |
| C25—H25—C2g | 1.00 | 2.61 | 3.413 (2) | 137 |
| C26—H26A—Cg3m | 0.98 | 2.87 | 3.682 (3) | 140 |
| C34B—H34E—Cg2m | 0.98 | 2.92 | 3.627 (9) | 130 |

Symmetry codes: (i) −x + 1, −y + 2, −z + 1; (ii) −x + 2, −y + 2, −z + 1; (iii) −x + 1, −y + 3, −z + 1; (iv) −x + 1, −y + 2, −z + 2; (v) −x + 1, y, z − 4.

and has an octahedral FeX₄N₄ (X = Br, Cl) coordination sphere. It is coordinated by the tertiary N atoms of four imidazole ligands [1-(2,6-disopropylphenyl)-1H-imidazole], in the equatorial plane, while the axial positions are occupied by the halogen ions. In (I), the axial Fe1—Cl1 bond length is 2.5356 (9) Å, while the equatorial Fe1—N1 and Fe1—N3 bond lengths are 2.188 (2) and 2.161 (2) Å, respectively. In the structures of compounds (II) and (IIb), the Fe—Br1 bond lengths are 2.7040 (5) and 2.7422 (3) Å, respectively. The Fe—N1 and Fe1—N3 bond lengths are 2.190 (3) and 2.161 (3) Å in (II), and 2.1889 (16) and 2.1789 (15) Å in (IIb). In each molecule, all of the imidazole C-bound H atoms are involved in intramolecular C—H···halogen hydrogen bonds (see Tables 1, 2 and 3).

In the two independent ligands of (I), the benzene rings (C4—C9 and C19—C24) are inclined to their attached imidazole rings (N1/N2/C1—C3 and N3/N4/C16—C18, respectively) by 88.19 (15) and 79.26 (14)°. In (II) and (IIb), the corresponding angles are 87.0 (3) and 79.2 (3)°, and 84.71 (11) and 80.58 (13)°, respectively. The imidazole rings (N1/N2/C1—C3 and N3/N4/C16—C18) of the two independent ligand molecules are inclined to one another by 70.04 (15), 69.3 (3) and 74.58 (14)° for clarity).
61.55 (12)$^\circ$ in (I), (II) and (IIb), respectively, while the benzene rings (C4–C9 and C19–C24) are inclined to one another by 82.83 (13), 83.0 (2) and 88.16 (12)$^\circ$, respectively. The various dihedral angles involving (IIb) differ slightly from those in (I) and (II) due to steric hindrance owing to the close proximity of the diethyl ether solvent molecule of crystallization.

### 3. Supramolecular features

In the crystal structures of all three compounds, (I), (II) and (IIb), molecules are linked via pairs of C–H···halogen hydrogen bonds, forming chains along the $a$ axis [(I) and (II)] and the $b$ axis, respectively, for (IIb) that enclose $R_2^2(12)$ ring motifs (Figs. 4, 5 and 6, respectively, and Tables 1, 2 and 3, respectively). They are linked by C–H···π interactions, forming sheets parallel to (001). In the crystal structure of compound (IIb), the diethyl ether solvent molecules are attached to the chains via C–H···O hydrogen bonds, and within the chains there are a series of C–H···π interactions present (Fig. 6 and Table 3).

### 4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update November 2013; Allen, 2002) indicated the presence of five tetrakis(N-substituted imidazole) iron halide complexes. Two of these involve iron(II), that is trans-dichloridotetrakis(5-chloro-1-methyl-1H-imidazole-N-iron(III)] chloride hydrate (Schröder et al., 2009) and trans-difluoridotetrakis(1-methylimidazole)iron(III) tetrafluoroborate (Christie et al., 1993). Two compounds containing aryl-substituted imidazoles where found, namely ($\mu_2$-oxido)-tetrachloridotetrakis(1-phenyl-1H-imidazole-N)diiiron(II) and ($\mu_2$-oxido)tetrachloridotetrakis[1-(2,6-disiopropylphenyl)-1H-imidazole-N]diiiron(II) (Schröder et al., 2009). The crystal structure of dichloridotetrakis(1-methylimidazole-N$^3$)iron(II) has also been reported (Reisner et al., 2007).

### 5. Synthesis and crystallization

The synthesis of the precursors bisimidazolium methylene tetrachlorido- and tetrabromidoferate(III) ([L1] and [L2], respectively, in Fig. 7) have been reported elsewhere (Mafua, 2006). Compound (I) was prepared as follows: to a solution of ([L1] 0.34 g, 0.5 mmol) in 20 ml of THF was added 0.09 g (2.3 mmol) of NaH 60% and 0.01 g (0.1 mmol) of 'BuOK, and the reaction mixture was heated at 340 K for 8 h. The solution was then filtered and the solvent evaporated under vacuum yielding an orange solid. Yellow crystals were obtained by slow diffusion of diethyl ether into a THF solution of the isolated orange solid. UV–vis (THF, 200–800 nm): 364, 290. Compounds (II) and (IIb) were prepared in a similar manner. To a solution of ([L2] 0.29 g, 0.5 mmol) in 20 ml of THF was added 0.09 g (2.3 mmol) of NaH 60% and 0.01 g (0.1 mmol) of 'BuOK at 273 K, and the reaction mixture was heated at reflux for 8 h. The solution was then filtered and the solvent evaporated under vacuum yielding a yellow–brown solid. Yellow crystals were obtained by slow diffusion of diethyl ether into a THF solution of the isolated orange solid. UV–vis (THF, 200–800 nm): 292. Two types of crystals were obtained: yellow plates for (II) and yellow blocks for (IIb).

### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. In all three compounds, the H atoms were included in calculated positions and treated as riding atoms: C–H = 0.95, 1.00 and 0.98 Å for CH(aromatic), CH and CH$_3$ H atoms, respectively, with $U_{iso}$(H) = 1.5$U_{eq}$(C-methyl) and = 1.2$U_{eq}$(C) for other H atoms. In (I) and (II), the methyl groups of an isopropyl group are disordered over two positions [occupancy ratio = 0.727 (13)/0.273 (13) in (I) and fixed at 0.50:0.5 for (II)]. In (IIb), one of the ethyl groups of the diethyl ether solvent molecule is disordered over two positions (occupancy ratio fixed at 0.50:0.5).
### Table 4
Experimental details.

|     | (I)                                      | (II)                                      | (IIIb)                                    |
|-----|-----------------------------------------|------------------------------------------|------------------------------------------|
| M   | [FeCl(H₂N₂)₃]                           | [FeBr₂(H₂N₂)₃]                           | [FeBr₂(C₁₀H₂₈N₄)₄]·2C₄H₁₀O               |
|     | 1040.07                                  | 1128.99                                  | 1277.22                                  |
| Crystal system, space group | Triclinic, P1                              | Triclinic, P1                             | Triclinic, P1                             |
| Temperature (K) | 173                                      | 173                                      | 173                                      |
| a, b, c (Å) | 8.877 (2), 12.628 (3), 13.810 (4)        | 9.0391 (11), 12.7658 (11), 13.689 (2)     | 11.6710 (8), 12.4758 (9), 13.5759 (10)   |
| α, β, γ (°) | 74.68 (2), 74.48 (2), 83.105 (18)       | 74.502 (9), 74.481 (12), 84.343 (9)      | 64.464 (5), 81.515 (6), 88.982 (6)       |
| V (Å³) | 1436.6 (7)                              | 1466.0 (3)                               | 1761.8 (2)                               |
| Z    | 1                                       | 1                                        | 1                                        |
| Radiation type | Mo K                                    | Mo K                                     | Mo K                                     |
| μ (mm⁻¹) | 0.40                                    | 1.66                                     | 1.39                                     |
| Crystal size (mm) | 0.25 × 0.20 × 0.15                     | 0.20 × 0.17 × 0.10                       | 0.50 × 0.50 × 0.50                      |
| Data collection |                                      |                                          |                                          |
| Diffractometer | Stoe IPDS 2                             | Stoe IPDS 2                              | Stoe IPDS 2                              |
| Absorption correction | Multi-scan (MULscanABS in   PLATON; Spek, 2009) | Multi-scan (MULscanABS in   PLATON; Spek, 2009) | Multi-scan (MULscanABS in   PLATON; Spek, 2009) |
| Tmin, Tmax | 0.966, 1.000                           | 0.457, 0.496                            | 0.557, 0.672                             |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 14618, 5214, 3012                      | 17613, 5312, 3013                       | 15799, 6374, 5714                      |
| Rint | 0.082                                   | 0.118                                   | 0.030                                   |
| (sin θ/λ)max (Å⁻¹) | 0.600                                   | 0.600                                   | 0.600                                   |
| Refinement |                                     |                                          |                                          |
| R(F²) = 2σ(F²), wR(F²), S | 0.043, 0.069, 0.80                      | 0.046, 0.081, 0.81                      | 0.031, 0.077, 1.03                      |
| No. of reflections | 5214                                   | 5312                                   | 6374                                    |
| No. of parameters | 339                                    | 350                                    | 378                                     |
| No. of restraints | 4                                      | 2                                      | 0                                       |
| H-atom treatment | H-atom parameters constrained         | H-atom parameters constrained          | H-atom parameters constrained          |
| Δρmax, Δρmin (e Å⁻³) | 0.23, −0.19                            | 0.59, −0.64                             | 0.44, −0.37                             |

Computer programs: X-AREA and X-RED32 (Stoe & Cie, 2006), SHELXS97 and SHELXL2013 (Sheldrick, 2008), PLATON (Spek, 2009), Mercury (Macrae et al., 2008) and pubCIF (Westrip, 2010).

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Crystal structures of trans-dichloridotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II), trans-dibromidotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II) and trans-dibromidotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II) diethyl ether disolvate

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Computing details

For all compounds, data collection: X-AREA (Stoe & Cie, 2006); cell refinement: X-AREA (Stoe & Cie, 2006); data reduction: X-RED32 (Stoe & Cie, 2006); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2013 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009) and Mercury (Macrae et al., 2008); software used to prepare material for publication: SHELXL2013 (Sheldrick, 2008), PLATON (Spek, 2009) and publCIF (Westrip, 2010).

(I) trans-Dichloridotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN³]iron(II)

Crystal data

\[\text{[FeCl}_2\text{C}_{15}\text{H}_{20}\text{N}_2\text{]}_4\]  
\(Z = 1\)  
\(F(000) = 556\)  
\(D_x = 1.202 \text{ Mg m}^{-3}\)  
\(\text{Mo Kα radiation, } \lambda = 0.71073 \text{ Å}\)  
Cell parameters from 7147 reflections  
\(\theta = 0.1–24.9°\)  
\(\mu = 0.40 \text{ mm}^{-1}\)  
\(T = 173 \text{ K}\)  
Block, colourless  
0.25 × 0.20 × 0.15 mm

Data collection

Stoe IPDS 2 diffractometer  
14618 measured reflections  
5214 independent reflections  
3012 reflections with \(I > 2\sigma(I)\)  
\(R_{int} = 0.082\)  
\(\theta_{\text{max}} = 25.3°, \theta_{\text{min}} = 1.6°\)  
\(h = -10→10\)  
\(k = -15→15\)  
\(l = -16→16\)
supporting information

**Refinement**

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.069$

$S = 0.80$

5214 reflections

339 parameters

4 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_c^2) + (0.0176P)^2]$

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

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

$\Delta\rho_{\text{max}} = 0.23 \, \text{e} \, \text{Å}^{-3}$

$\Delta\rho_{\text{min}} = -0.19 \, \text{e} \, \text{Å}^{-3}$

**Special details**

**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.

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

|          | $x$    | $y$    | $z$    | $U_{eq}$ | Occ. (<1) |
|----------|--------|--------|--------|----------|-----------|
| Fe1      | 0.5000 | 0.0000 | 0.5000 | 0.02088 (16) |
| Cl1      | 0.70366 (8) | -0.15905 (5) | 0.50114 (5) | 0.02791 (18) |
| N1       | 0.5146 (2) | 0.01056 (16) | 0.33706 (16) | 0.0268 (5) |
| N2       | 0.4532 (3) | 0.06854 (17) | 0.18661 (15) | 0.0276 (5) |
| N3       | 0.3206 (2) | -0.11518 (16) | 0.53380 (15) | 0.0242 (5) |
| N4       | 0.2109 (2) | -0.26733 (16) | 0.54788 (16) | 0.0253 (5) |
| C1       | 0.4309 (3) | 0.0828 (2) | 0.28262 (19) | 0.0272 (7) |
| H1       | 0.3626 | 0.1386 | 0.3081 | 0.033* |
| C2       | 0.5931 (3) | -0.0546 (2) | 0.2729 (2) | 0.0353 (7) |
| H2       | 0.6631 | -0.1152 | 0.2910 | 0.042* |
| C3       | 0.5573 (3) | -0.0208 (2) | 0.1802 (2) | 0.0364 (7) |
| H3       | 0.5960 | -0.0522 | 0.1223 | 0.044* |
| C4       | 0.3853 (3) | 0.1369 (2) | 0.10628 (19) | 0.0287 (7) |
| C5       | 0.2450 (3) | 0.1095 (2) | 0.09679 (19) | 0.0326 (7) |
| C6       | 0.1819 (4) | 0.1781 (2) | 0.0180 (2) | 0.0435 (8) |
| H6       | 0.0857 | 0.1619 | 0.0087 | 0.052* |
| C7       | 0.2585 (4) | 0.2685 (3) | -0.0459 (2) | 0.0500 (9) |
| H7       | 0.2158 | 0.3134 | -0.1001 | 0.060* |
| C8       | 0.3955 (4) | 0.2953 (2) | -0.0330 (2) | 0.0474 (8) |
| H8       | 0.4447 | 0.3595 | -0.0772 | 0.057* |
| C9       | 0.4638 (3) | 0.2302 (2) | 0.0439 (2) | 0.0355 (7) |
| C10      | 0.1572 (4) | 0.0119 (2) | 0.1701 (2) | 0.0423 (8) |
| H10A     | 0.2349 | -0.0377 | 0.2039 | 0.051* | 0.727 (13) |
| H10B     | 0.2081 | -0.0198 | 0.2287 | 0.051* | 0.273 (13) |
| C11A     | 0.0312 (9) | 0.0456 (5) | 0.2559 (6) | 0.0590 (19) | 0.727 (13) |
| H11A     | 0.0779 | 0.0835 | 0.2933 | 0.088* | 0.727 (13) |
| H11B     | -0.0186 | -0.0199 | 0.3039 | 0.088* | 0.727 (13) |
| H11C     | -0.0475 | 0.0951 | 0.2262 | 0.088* | 0.727 (13) |

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sup-2
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C12A | 0.0892 (13) | −0.0560 (8) | 0.1187 (8) | 0.078 (3) | 0.727 (13) |
| H12A | 0.0538 | −0.1247 | 0.1687 | 0.117* | 0.727 (13) |
| H12B | 0.1694 | −0.0728 | 0.0598 | 0.117* | 0.727 (13) |
| H12C | 0.0002 | −0.0146 | 0.0944 | 0.117* | 0.727 (13) |
| C11B | −0.0112 (19) | 0.0578 (14) | 0.2122 (15) | 0.0590 (19) | 0.273 (13) |
| H11D | −0.0654 | 0.0800 | 0.1562 | 0.088* | 0.273 (13) |
| H11E | −0.0058 | 0.1216 | 0.2387 | 0.088* | 0.273 (13) |
| H11F | −0.0687 | 0.0008 | 0.2682 | 0.088* | 0.273 (13) |
| C12B | 0.159 (4) | −0.073 (2) | 0.112 (3) | 0.078 (3) | 0.273 (13) |
| H12D | 0.1249 | −0.0384 | 0.0489 | 0.117* | 0.273 (13) |
| H12E | 0.0880 | −0.1302 | 0.1559 | 0.117* | 0.273 (13) |
| H12F | 0.2656 | −0.1056 | 0.0946 | 0.117* | 0.273 (13) |
| C13 | 0.6097 (4) | 0.2615 (2) | 0.0631 (2) | 0.0444 (8) |
| H13 | 0.6631 | 0.1923 | 0.0958 | 0.053* |
| C14 | 0.5694 (4) | 0.3354 (3) | 0.1394 (3) | 0.0716 (11) |
| H14A | 0.5236 | 0.4063 | 0.1075 | 0.086* |
| H14B | 0.6648 | 0.3473 | 0.1572 | 0.086* |
| H14C | 0.4939 | 0.3000 | 0.2024 | 0.086* |
| C15 | 0.7269 (4) | 0.3182 (3) | −0.0346 (3) | 0.0669 (11) |
| H15A | 0.7469 | 0.2747 | −0.0863 | 0.080* |
| H15B | 0.8251 | 0.3247 | −0.0174 | 0.080* |
| H15C | 0.6839 | 0.3917 | −0.0626 | 0.080* |
| C16 | 0.3362 (3) | −0.2225 (2) | 0.55469 (18) | 0.0253 (6) |
| H16 | 0.4257 | −0.2639 | 0.5726 | 0.030* |
| C17 | 0.1766 (3) | −0.0894 (2) | 0.5126 (2) | 0.0301 (7) |
| H17 | 0.1321 | −0.0168 | 0.4946 | 0.036* |
| C18 | 0.1064 (3) | −0.1826 (2) | 0.5210 (2) | 0.0308 (7) |
| H18 | 0.0063 | −0.1879 | 0.5105 | 0.037* |
| C19 | 0.1907 (3) | −0.38269 (19) | 0.5634 (2) | 0.0259 (6) |
| C20 | 0.2662 (3) | −0.4342 (2) | 0.4836 (2) | 0.0309 (7) |
| C21 | 0.2407 (3) | −0.5445 (2) | 0.5010 (2) | 0.0385 (7) |
| H21 | 0.2882 | −0.5822 | 0.4484 | 0.046* |
| C22 | 0.1479 (4) | −0.6007 (2) | 0.5928 (2) | 0.0450 (8) |
| H22 | 0.1314 | −0.6762 | 0.6027 | 0.054* |
| C23 | 0.0796 (3) | −0.5482 (2) | 0.6698 (2) | 0.0381 (7) |
| H23 | 0.0175 | −0.5885 | 0.7332 | 0.046* |
| C24 | 0.0987 (3) | −0.4372 (2) | 0.6576 (2) | 0.0292 (6) |
| C25 | 0.3709 (3) | −0.3722 (2) | 0.3836 (2) | 0.0350 (7) |
| H25 | 0.4332 | −0.3231 | 0.4023 | 0.042* |
| C26 | 0.2778 (4) | −0.2999 (3) | 0.3121 (2) | 0.0568 (10) |
| H26A | 0.2138 | −0.3454 | 0.2931 | 0.068* |
| H26B | 0.3494 | −0.2599 | 0.2494 | 0.068* |
| H26C | 0.2095 | −0.2472 | 0.3472 | 0.068* |
| C27 | 0.4861 (4) | −0.4467 (3) | 0.3262 (2) | 0.0492 (9) |
| H27C | 0.5622 | −0.4022 | 0.2696 | 0.059* |
| H27B | 0.4297 | −0.4885 | 0.2979 | 0.059* |
| H27A | 0.5410 | −0.4977 | 0.3741 | 0.059* |
| C28 | 0.0214 (3) | −0.3808 (2) | 0.7438 (2) | 0.0333 (7) |
## Atomic displacement parameters (Å²)

|      | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$   | $U^{23}$   |
|------|------------|------------|------------|------------|------------|------------|
| Fe1  | 0.0218 (4) | 0.0163 (3) | 0.0257 (3) | −0.0025 (3)| −0.0081 (3)| −0.0043 (3)|
| Cl1  | 0.0265 (4) | 0.0220 (4) | 0.0379 (4) | 0.0027 (3) | −0.0120 (3)| −0.0093 (3)|
| N1   | 0.0268 (4) | 0.0244 (12)| 0.0299 (12)| 0.0021 (10)| −0.0099 (10)| −0.0066 (10)|
| N2   | 0.0325 (14)| 0.0284 (12)| 0.0217 (12)| 0.0013 (11)| −0.0088 (10)| −0.0047 (10)|
| N3   | 0.0211 (13)| 0.0185 (12)| 0.0329 (12)| −0.0032 (9)| −0.0086 (10)| −0.0030 (10)|
| N4   | 0.0213 (13)| 0.0189 (11)| 0.0373 (13)| −0.0039 (10)| −0.0096 (10)| −0.0062 (10)|
| C1   | 0.0306 (17)| 0.0260 (15)| 0.0248 (15)| 0.0020 (13)| −0.0061 (13)| −0.0080 (12)|
| C2   | 0.0389 (19)| 0.0299 (16)| 0.0362 (17)| 0.0103 (14)| −0.0113 (14)| −0.0095 (14)|
| C3   | 0.045 (2)  | 0.0317 (16)| 0.0340 (17)| 0.0107 (15)| −0.0116 (14)| −0.0141 (13)|
| C4   | 0.0371 (18)| 0.0250 (15)| 0.0231 (15)| 0.0061 (13)| −0.0082 (13)| −0.0069 (12)|
| C5   | 0.0391 (19)| 0.0339 (16)| 0.0271 (15)| 0.0023 (14)| −0.0090 (14)| −0.0121 (13)|
| C6   | 0.045 (2)  | 0.050 (2)  | 0.0411 (18)| 0.0104 (16)| −0.0220 (16)| −0.0140 (16)|
| C7   | 0.069 (3)  | 0.044 (2)  | 0.0357 (18)| 0.0143 (18)| −0.0220 (18)| −0.0054 (16)|
| C8   | 0.064 (2)  | 0.0342 (18)| 0.0362 (18)| −0.0012 (17)| −0.0106 (17)| 0.0024 (14)|
| C9   | 0.0412 (19)| 0.0334 (17)| 0.0276 (15)| −0.0013 (14)| −0.0012 (14)| −0.0074 (13)|
| C10  | 0.045 (2)  | 0.0419 (18)| 0.0443 (18)| −0.0084 (15)| −0.0189 (16)| −0.0069 (15)|
| C11A | 0.076 (4)  | 0.051 (3)  | 0.041 (4)  | −0.019 (3) | 0.001 (3)  | −0.006 (3)  |
| C12A | 0.112 (10)| 0.050 (4)  | 0.073 (3)  | −0.019 (5) | −0.008 (7) | −0.025 (3) |
| C11B | 0.076 (4)  | 0.051 (3)  | 0.041 (4)  | −0.019 (3) | 0.001 (3)  | −0.006 (3)  |
| C12B | 0.112 (10)| 0.050 (4)  | 0.073 (3)  | −0.019 (5) | −0.008 (7) | −0.025 (3) |
| C13  | 0.046 (2)  | 0.0368 (18)| 0.0445 (19)| −0.0098 (15)| −0.0051 (16)| −0.0018 (15)|
| C14  | 0.060 (3)  | 0.074 (3)  | 0.089 (3)  | −0.027 (2) | −0.007 (2) | −0.035 (2)  |
| C15  | 0.059 (3)  | 0.064 (2)  | 0.064 (2)  | −0.014 (2) | 0.001 (2)  | −0.0027 (19)|
| C16  | 0.0206 (16)| 0.0251 (15)| 0.0303 (16)| −0.0025 (12)| −0.0099 (13)| −0.0026 (12)|
| C17  | 0.0248 (16)| 0.0184 (14)| 0.0446 (17)| 0.0005 (12)| −0.0095 (14)| −0.0032 (12)|
| C18  | 0.0214 (16)| 0.0219 (15)| 0.0510 (18)| 0.0021 (12)| −0.0145 (14)| −0.0077 (13)|
| C19  | 0.0239 (16)| 0.0168 (13)| 0.0410 (16)| −0.0021 (12)| −0.0127 (13)| −0.0084 (12)|
| C20  | 0.0285 (17)| 0.0274 (15)| 0.0386 (16)| −0.0017 (12)| −0.0094 (13)| −0.0097 (13)|
| C21  | 0.041 (2)  | 0.0302 (17)| 0.0468 (19)| −0.0017 (14)| −0.0055 (16)| −0.0195 (14)|
| C22  | 0.052 (2)  | 0.0234 (16)| 0.059 (2)  | −0.0089 (15)| −0.0063 (18)| −0.0134 (15)|
| C23  | 0.041 (2)  | 0.0232 (16)| 0.0449 (18)| −0.0090 (14)| 0.0001 (15) | −0.0074 (14)|
| C24  | 0.0247 (16)| 0.0211 (14)| 0.0395 (16)| −0.0043 (12)| −0.0061 (13)| −0.0042 (12)|
| C25  | 0.0353 (18)| 0.0357 (17)| 0.0360 (16)| −0.0063 (13)| −0.0062 (14)| −0.0127 (13)|
| C26  | 0.056 (2)  | 0.057 (2)  | 0.046 (2)  | 0.0057 (19) | −0.0088 (18)| −0.0019 (17)|
| C27  | 0.042 (2)  | 0.061 (2)  | 0.0399 (19)| 0.0060 (17)| −0.0046 (16)| −0.0137 (17)|
Geometric parameters (Å, °)

|       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|
| Fe1—N3       | 2.161 (2) | C12B—H12D       | 0.980       |
| Fe1—N3       | 2.161 (2) | C12B—H12E       | 0.980       |
| Fe1—N1       | 2.188 (2) | C12B—H12F       | 0.980       |
| Fe1—N1       | 2.188 (2) | C13—C15         | 1.527 (4)   |
| Fe1—Cl1      | 2.5356 (9) | C13—C14         | 1.532 (4)   |
| Fe1—Cl1      | 2.5356 (9) | C13—H13         | 1.0000      |
| N1—C1        | 1.313 (3) | C14—H14A        | 0.980       |
| N1—C2        | 1.365 (3) | C14—H14B        | 0.980       |
| N2—C1        | 1.344 (3) | C14—H14C        | 0.980       |
| N2—C3        | 1.376 (3) | C15—H15A        | 0.980       |
| N2—C4        | 1.437 (3) | C15—H15B        | 0.980       |
| N3—C16       | 1.307 (3) | C15—H15C        | 0.980       |
| N3—C17       | 1.369 (3) | C16—H16         | 0.9500      |
| N4—C16       | 1.342 (3) | C17—C18         | 1.362 (4)   |
| N4—C18       | 1.371 (3) | C17—H17         | 0.9500      |
| N4—C19       | 1.441 (3) | C18—H18         | 0.9500      |
| C1—H1        | 0.9500   | C19—C24         | 1.387 (4)   |
| C2—C3        | 1.349 (4) | C19—C20         | 1.403 (4)   |
| C2—H2        | 0.9500   | C20—C21         | 1.385 (4)   |
| C3—H3        | 0.9500   | C20—C25         | 1.517 (4)   |
| C4—C5        | 1.379 (4) | C21—C22         | 1.377 (4)   |
| C4—C9        | 1.399 (4) | C21—H21         | 0.9500      |
| C5—C6        | 1.400 (3) | C22—C23         | 1.367 (4)   |
| C5—C10       | 1.517 (4) | C22—H22         | 0.9500      |
| C6—C7        | 1.370 (4) | C23—C24         | 1.393 (4)   |
| C6—H6        | 0.9500   | C23—H23         | 0.9500      |
| C7—C8        | 1.368 (4) | C24—C28         | 1.512 (4)   |
| C7—H7        | 0.9500   | C25—C26         | 1.508 (4)   |
| C8—C9        | 1.390 (4) | C25—C27         | 1.513 (4)   |
| C8—H8        | 0.9500   | C25—H25         | 1.0000      |
| C9—C13       | 1.505 (4) | C26—H26A        | 0.9800      |
| C10—C12B     | 1.489 (17)| C26—H26B        | 0.9800      |
| C10—C11A     | 1.509 (6) | C26—H26C        | 0.9800      |
| C10—C12A     | 1.509 (8) | C27—H27C        | 0.9800      |
| C10—C11B     | 1.553 (14)| C27—H27B        | 0.9800      |
| C10—H10A     | 1.0000   | C27—H27A        | 0.9800      |
| C10—H10B     | 1.0000   | C28—C30         | 1.515 (4)   |
| C11A—H11A    | 0.9800   | C28—C29         | 1.522 (4)   |
| C11A—H11B    | 0.9800   | C28—H28         | 1.0000      |
| C11A—H11C    | 0.9800   | C29—H29A        | 0.9800      |
| C12A—H12A    | 0.9800   | C29—H29B        | 0.9800      |
| C12A—H12B    | 0.9800   | C29—H29C        | 0.9800      |
C12A—H12C 0.9800 C30—H30C 0.9800
C11B—H11D 0.9800 C30—H30B 0.9800
C11B—H11E 0.9800 C30—H30A 0.9800
C11B—H11F 0.9800

N3—Fe1—N3i 180.0 H12D—C12B—H12E 109.5
N3—Fe1—N1 85.67 (8) C10—C12B—H12F 109.5
N3—Fe1—N1i 94.33 (8) H12D—C12B—H12F 109.5
N1—Fe1—N1i 85.67 (8) C9—C13—C15 114.4 (3)
N1—Fe1—N1i 180.0 C9—C13—C14 111.1 (3)
N3—Fe1—Cl1 89.14 (6) C15—C13—C14 108.7 (3)
N3—Fe1—Cl1 90.86 (6) C9—C13—H13 107.5
N1—Fe1—Cl1 90.37 (6) C15—C13—H13 107.5
N1—Fe1—Cl1i 89.63 (6) C13—C14—H14A 109.5
N3—Fe1—Cl1i 90.86 (6) C13—C14—H14B 109.5
N1—Fe1—Cl1i 90.37 (6) C13—C14—H14C 109.5
C1—N1—C2 105.1 (2) H14A—C14—H14B 109.5
C1—N1—Fe1 123.17 (17) C13—C14—H14C 109.5
C2—N1—Fe1 131.53 (16) N3—C16—N4 112.0 (2)
C1—N2—C3 106.4 (2) C16—N3—Fe1 125.16 (16) N3—C16—H16 124.0
C1—N2—C4 126.0 (2) N4—C16—H16 124.0
C3—N2—C4 127.5 (2) C18—C17—N3 110.3 (2)
C16—N3—C17 105.2 (2) C18—C17—H17 124.9
C16—N3—Fe1 127.93 (17) N3—C16—N4i 112.0 (2)
C17—N3—Fe1 125.16 (16) N3—C16—H16 124.0
C16—N4—C18 107.2 (2) N4—C16—H16 124.0
C16—N4—C19 126.7 (2) C18—C17—N3i 124.9
C18—N4—C19i 126.1 (2) C18—C17—H17 124.9
N1—C1—N2 112.1 (2) N3—C17—H17 124.9
N1—C1—H1 124.0 C17—C18—N4 105.3 (2)
N2—C1—H1 124.0 C17—C18—H18 127.4
C3—C2—N1 110.5 (2) N4—C18—H18 127.4
C3—C2—H2 124.8 C24—C19—C20 123.5 (2)
N1—C2—H2 124.8 C24—C19—N4 117.9 (2)
C2—C3—N2 105.9 (2) C20—C19—N4 118.5 (2)
C2—C3—H3 127.0 C21—C20—C19 116.6 (2)
N2—C3—H3 127.0 C21—C20—C25 121.9 (3)
C5—C4—C9 123.6 (2) C19—C20—C25 121.6 (2)
C5—C4—N2 118.8 (2) C22—C21—C20 121.5 (3)
C9—C4—N2 117.5 (3) C22—C21—H21 119.3
C4—C5—C6 117.3 (3) C20—C21—H21 119.3
C4—C5—C10 122.4 (2) C23—C22—C21 120.2 (3)
C6—C5—C10 120.3 (3) C23—C22—H22 119.9
C7—C6—C5 120.2 (3) C21—C22—H22 119.9
| Bond          | Angle (°)         | Bond          | Angle (°)         | Bond          | Angle (°)         |
|---------------|------------------|---------------|------------------|---------------|------------------|
| C7—C6—H6     | 119.9            | C22—C23—C24  | 121.7 (3)        |
| C5—C6—H6     | 119.9            | C22—C23—H23  | 119.2            |
| C8—C7—C6     | 121.2 (3)        | C24—C23—H23  | 119.2            |
| C8—C7—H7     | 119.4            | C19—C24—C23  | 116.6 (3)        |
| C6—C7—H7     | 119.4            | C19—C24—C28  | 122.7 (2)        |
| C7—C8—C9     | 121.1 (3)        | C23—C24—C28  | 120.7 (2)        |
| C7—C8—H8     | 119.4            | C26—C25—C27  | 109.4 (2)        |
| C9—C8—H8     | 119.4            | C26—C25—C20  | 112.0 (2)        |
| C8—C9—C4     | 116.5 (3)        | C27—C25—C20  | 113.2 (2)        |
| C8—C9—C13    | 122.0 (3)        | C26—C25—H25  | 107.3            |
| C4—C9—C13    | 121.5 (2)        | C27—C25—H25  | 107.3            |
| C12B—C10—C5  | 109.1 (14)       | C20—C25—H25  | 107.3            |
| C11A—C10—C5  | 111.8 (3)        | C25—C26—H26A | 109.5            |
| C11A—C10—C12A| 109.9 (4)        | C25—C26—H26B | 109.5            |
| C5—C10—C12A  | 114.9 (5)        | H26A—C26—H26B| 109.5            |
| C12B—C10—C11B| 112.4 (13)       | C25—C26—H26C | 109.5            |
| C5—C10—C11B  | 105.9 (7)        | H26A—C26—H26C| 109.5            |
| C11A—C10—H10A| 106.6            | H26B—C26—H26C| 109.5            |
| C5—C10—H10A  | 106.6            | C25—C27—H27C | 109.5            |
| C12A—C10—H10A| 106.6            | C25—C27—H27B | 109.5            |
| C12B—C10—H10B| 109.8            | H27C—C27—H27B| 109.5            |
| C5—C10—H10B  | 109.8            | C25—C27—H27A | 109.5            |
| C11B—C10—H10B| 109.8            | H27C—C27—H27A| 109.5            |
| C10—C11A—H11A| 109.5            | H27B—C27—H27A| 109.5            |
| C10—C11A—H11B| 109.5            | C24—C28—C30  | 110.7 (2)        |
| H11A—C11A—H11B| 109.5           | C24—C28—C29  | 112.6 (2)        |
| C10—C11A—H11C| 109.5            | C30—C28—C29  | 110.6 (2)        |
| H11A—C11A—H11C| 109.5           | C24—C28—H28  | 107.6            |
| H11B—C11A—H11C| 109.5           | C30—C28—H28  | 107.6            |
| C10—C12A—H12A| 109.5            | C29—C28—H28  | 107.6            |
| C10—C12A—H12B| 109.5            | C28—C29—H29A | 109.5            |
| H12A—C12A—H12B| 109.5           | C28—C29—H29B | 109.5            |
| C10—C12A—H12C| 109.5            | H29A—C29—H29B| 109.5            |
| H12A—C12A—H12C| 109.5           | C28—C29—H29C | 109.5            |
| H12B—C12A—H12C| 109.5           | H29A—C29—H29C| 109.5            |
| C10—C11B—H11D| 109.5            | H29B—C29—H29C| 109.5            |
| C10—C11B—H11E| 109.5            | C28—C30—H30C | 109.5            |
| H11D—C11B—H11E| 109.5           | C28—C30—H30B | 109.5            |
| C10—C11B—H11F| 109.5            | H30C—C30—H30B| 109.5            |
| H11E—C11B—H11F| 109.5           | C28—C30—H30A | 109.5            |
| C10—C12B—H12D| 109.5            | H30C—C30—H30A| 109.5            |
| C10—C12B—H12E| 109.5            | H30B—C30—H30A| 109.5            |
| C2—N1—C1—N2  | −0.9 (3)         | C8—C9—C13—C14| 87.8 (3)         |
| Fe1—N1—C1—N2 | −176.06 (17)     | C4—C9—C13—C14| −88.7 (3)        |
| C3—N2—C1—N1  | 1.0 (3)          | C17—N3—C16—N4| 0.2 (3)          |
| C4—N2—C1—N1  | −176.7 (2)       | Fe1—N3—C16—N4| −165.34 (16)     |

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C1—N1—C2—C3  0.5 (3)  C18—N4—C16—N3  −0.3 (3)
C1—N1—C2—C3  175.1 (2)  C19—N4—C18—C17  −178.5 (2)
N1—C2—C3—N2  0.1 (3)  C16—N4—C19—C24  101.2 (3)
C1—N2—C4—C5  −0.6 (3)  C16—N4—C19—C20  100.5 (3)
C3—N2—C4—C5  177.1 (3)  C18—N4—C19—C20  −177.5 (2)
C9—C4—C5—C6  1.9 (5)  C19—N4—C18—C17  101.2 (3)
N2—C4—C5—C6  179.8 (2)  C19—N4—C18—C17  −178.5 (2)
C9—C4—C5—C10  −175.9 (3)  C16—N4—C19—C24  101.2 (3)
C3—N2—C4—C9  86.0 (3)  C16—N4—C19—C20  100.5 (3)
C1—N2—C4—C9  −92.0 (3)  C16—N4—C19—C24  101.2 (3)
C4—C5—C6—C7  1.9 (4)  C16—N4—C19—C20  100.5 (3)
C5—C4—C9—C8  −1.8 (4)  C16—N4—C19—C24  101.2 (3)
C5—C4—C9—C13  174.8 (3)  C16—N4—C19—C20  100.5 (3)
N2—C4—C9—C8  −91.3 (3)  C16—N4—C19—C24  101.2 (3)
N2—C4—C9—C13  179.7 (2)  C16—N4—C19—C20  100.5 (3)
C4—C5—C10—C12B  −112.5 (13)  C22—C23—C24—C19  102.9 (3)
C6—C5—C10—C12B  69.8 (14)  C22—C23—C24—C19  179.8 (3)
C4—C5—C10—C11A  96.3 (5)  C22—C23—C24—C19  0.0 (4)
C6—C5—C10—C11A  −81.4 (5)  C22—C23—C24—C19  102.9 (3)
C4—C5—C10—C12A  −137.6 (5)  C22—C23—C24—C19  179.8 (3)
C6—C5—C10—C12A  44.7 (6)  C22—C23—C24—C19  0.0 (4)
C4—C5—C10—C11B  126.4 (9)  C22—C23—C24—C19  179.8 (3)
C6—C5—C10—C11B  −51.4 (9)  C22—C23—C24—C19  0.0 (4)
C8—C9—C13—C15  −35.7 (4)  C22—C23—C24—C19  179.8 (3)
C4—C9—C13—C15  147.8 (3)  C22—C23—C24—C19  179.8 (3)

Symmetry code: (i) −x+1, −y, −z+1.

Hydrogen-bond geometry (Å, °)

Cg3 and Cg4 are the centroids of rings C4–C9 and C19–C24, respectively.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|------|-------|---------|
| C1—H1···C11i | 0.95 | 2.62 | 3.257 (3) | 125 |
| C2—H2···C11 | 0.95 | 2.92 | 3.433 (3) | 115 |
| C16—H16···C11 | 0.95 | 2.76 | 3.294 (3) | 117 |
| C17—H17···C11 | 0.95 | 2.82 | 3.375 (3) | 118 |
| C18—H18···C11a | 0.95 | 2.70 | 3.629 (3) | 166 |
| C27—H27A···Cg4ii | 0.98 | 2.79 | 3.562 (4) | 136 |
| C30—H30C···Cg3v | 0.98 | 2.92 | 3.901 (4) | 176 |

Symmetry codes: (i) −x+1, −y, −z+1; (ii) x+1, y, z; (iii) −x+1, −y, −z+1; (iv) −x, −y, −z+1.
(II) *trans*-Dibromidotetrakis[1-(2,6-diisopropylphenyl)-1*H*-imidazole-κ*N*3]iron(II)

**Crystal data**

\[ \text{[FeBr}_2(\text{C}_{15}\text{H}_{20}\text{N}_2)_4] } \]

- \( M_r = 1128.99 \)
- Triclinic, \( P\overline{1} \)
- Hall symbol: -P 1
- \( a = 9.0391 \) (11) Å
- \( b = 12.7658 \) (11) Å
- \( c = 13.689 \) (2) Å
- \( \alpha = 74.502 \) (9)°
- \( \beta = 74.481 \) (12)°
- \( \gamma = 84.343 \) (9)°
- \( V = 1466.0 \) (3) Å³
- \( Z = 1 \)
- \( F(000) = 592 \)
- \( D_x = 1.279 \) Mg m⁻³
- Mo \( K\alpha \) radiation, \( \lambda = 0.71073 \) Å
- Cell parameters from 7257 reflections
- \( \theta = 0.1–24.9\degree \)
- \( \mu = 1.66 \) mm⁻¹
- \( T = 173 \) K
- Plate, yellow

**Data collection**

- Stoe IPDS 2 diffractometer
- Radiation source: fine-focus sealed tube
- Plane graphite monochromator
- \( \phi + \omega \) scans
- Absorption correction: multi-scan
- (MULscanABS in PLATON; Spek, 2009)
- \( T_{\text{min}} = 0.457, T_{\text{max}} = 0.496 \)
- 17613 measured reflections
- 5312 independent reflections
- 3013 reflections with \( I > 2 \sigma(I) \)
- \( R_{int} = 0.118 \)
- \( \theta_{\text{max}} = 25.2\degree, \theta_{\text{min}} = 1.6\degree \)
- \( h = -10 \rightarrow 10 \)
- \( k = -15 \rightarrow 15 \)
- \( l = -16 \rightarrow 16 \)

**Refinement**

- Refinement on \( F^2 \)
- Least-squares matrix: full
- \( R[F^2 > 2 \sigma(F^2)] = 0.046 \)
- \( wR(F^2) = 0.081 \)
- \( S = 0.81 \)
- 5312 reflections
- 350 parameters
- 2 restraints

Hydrogen site location: inferred from neighbouring sites

- H-atom parameters constrained

\( \Delta \rho_{\text{max}} = 0.59 \) e Å⁻³
\( \Delta \rho_{\text{min}} = -0.64 \) e Å⁻³

**Special details**

**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.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)**

|     | \( x \)  | \( y \)  | \( z \)  | \( U_{eq} \) |
|-----|---------|---------|---------|-----------|
| Fe1 | 0.5000  | 0.0000  | 0.5000  | 0.0194 (2) |
| Br1 | 0.70958 (6) | −0.16630 (4) | 0.49630 (4) | 0.02557 (14) |
| N1  | 0.5093 (4) | 0.0144 (3)  | 0.3354 (3) | 0.0234 (8)  |
| N2  | 0.4486 (4) | 0.0707 (3)  | 0.1838 (3) | 0.0260 (9)  |
| N3  | 0.3197 (4) | −0.1141 (2) | 0.5363 (3) | 0.0203 (8)  |
| N4  | 0.2095 (4) | −0.2665 (3) | 0.5529 (3) | 0.0238 (8)  |
| C1  | 0.4300 (5) | 0.0853 (3)  | 0.2808 (3) | 0.0265 (11) |
| H1  | 0.3663  | 0.1411   | 0.3060  | 0.032*     |
| C2  | 0.5844 (6) | −0.0508 (4) | 0.2709 (4) | 0.0356 (13) |
### Supporting Information

| Atom | U1    | U2    | U3    | U1-U2 | U1-U3 | U2-U3 | U1-U2-U3 | U1-U3-U2 | U2-U3-U1 | U1-U2-U3-U4 |
|------|-------|-------|-------|-------|-------|-------|-----------|-----------|-----------|-------------|
| H2   | 0.6517| -0.1106| 0.2890| 0.043*| 0.0362| 0.12 |
| C3   | 0.5470 (5)| -0.0162 (4)| 0.1766 (4)| 0.0288| 0.0307| 0.11 |
| H3   | 0.5827| -0.0467| 0.1180| 0.043*| 0.0362| 0.12 |
| C4   | 0.3836 (6)| 0.1393 (4)| 0.1024 (3)| 0.0288| 0.0307| 0.11 |
| C5   | 0.2450 (5)| 0.1109 (3)| 0.0933 (3)| 0.0288| 0.0307| 0.11 |
| C6   | 0.1847 (6)| 0.1782 (4)| 0.0137 (4)| 0.0288| 0.0307| 0.11 |
| H6   | 0.0900| 0.1615| 0.0046| 0.051*| 0.0362| 0.12 |
| C7   | 0.2617 (7)| 0.2686 (4)| -0.0516 (4)| 0.0457| 0.0307| 0.11 |
| H7   | 0.2213| 0.3127| -0.1068| 0.055*| 0.0362| 0.12 |
| C8   | 0.3959 (6)| 0.2954 (4)| -0.0377 (4)| 0.0448| 0.0307| 0.11 |
| H8   | 0.4459| 0.3592| -0.0828| 0.054*| 0.0362| 0.12 |
| C9   | 0.4613 (5)| 0.2325 (4)| 0.0401 (4)| 0.0337| 0.0307| 0.11 |
| C10  | 0.1572 (6)| 0.0135 (4)| 0.1677 (4)| 0.0426| 0.0307| 0.11 |
| H10A | 0.2393| -0.0198| 0.2040| 0.051*| 0.0307| 0.11 |
| H10B | 0.2132| -0.0342| 0.2179| 0.051*| 0.0307| 0.11 |
| C11A | 0.041 (2)| 0.0434 (18)| 0.2621 (10)| 0.051*| 0.0307| 0.11 |
| H11A | 0.0954| 0.0745| 0.3004| 0.061*| 0.0307| 0.11 |
| H11B | -0.0110| -0.0222| 0.3087| 0.061*| 0.0307| 0.11 |
| H11C | -0.0349| 0.0967| 0.2373| 0.061*| 0.0307| 0.11 |
| C12A | 0.153 (2)| -0.0733 (15)| 0.1164 (19)| 0.079 (6)| 0.0307| 0.11 |
| H12A | 0.1077| -0.0442| 0.0565| 0.095*| 0.0307| 0.11 |
| H12B | 0.0900| -0.1325| 0.1664| 0.095*| 0.0307| 0.11 |
| H12C | 0.2573| -0.1012| 0.0920| 0.095*| 0.0307| 0.11 |
| C11B | 0.001 (2)| 0.0529 (19)| 0.2171 (14)| 0.100 (9)| 0.0307| 0.11 |
| H11D | 0.0113| 0.1088| 0.2518| 0.119*| 0.0307| 0.11 |
| H11E | -0.0553| -0.0081| 0.2689| 0.119*| 0.0307| 0.11 |
| H11F | -0.0544| 0.0838| 0.1631| 0.119*| 0.0307| 0.11 |
| C12B | 0.077 (2)| -0.0471 (16)| 0.1146 (18)| 0.059 (5)| 0.0307| 0.11 |
| C12D | 0.0408| -0.1168| 0.1629| 0.070*| 0.0307| 0.11 |
| H12E | 0.1487| -0.0603| 0.0512| 0.070*| 0.0307| 0.11 |
| H12F | -0.0115| -0.0030| 0.0957| 0.070*| 0.0307| 0.11 |
| C13  | 0.6051 (6)| 0.2642 (4)| 0.0597 (4)| 0.0441 (13)| 0.0307| 0.11 |
| H13  | 0.6536| 0.1964| 0.0959| 0.053*| 0.0307| 0.11 |
| C14  | 0.5652 (7)| 0.3400 (5)| 0.1332 (5)| 0.077 (2)| 0.0307| 0.11 |
| H14A | 0.5271| 0.4103| 0.0971| 0.093*| 0.0307| 0.11 |
| H14B | 0.6573| 0.3508| 0.1538| 0.093*| 0.0307| 0.11 |
| H14C | 0.4857| 0.3075| 0.1957| 0.093*| 0.0307| 0.11 |
| C15  | 0.7247 (7)| 0.3167 (5)| -0.0404 (5)| 0.075 (2)| 0.0307| 0.11 |
| H15A | 0.7432| 0.2709| -0.0898| 0.090*| 0.0307| 0.11 |
| H15B | 0.8208| 0.3241| -0.0229| 0.090*| 0.0307| 0.11 |
| H15C | 0.6863| 0.3887| -0.0723| 0.090*| 0.0307| 0.11 |
| C16  | 0.3330 (5)| -0.2203 (3)| 0.5594 (3)| 0.0246 (10)| 0.0307| 0.11 |
| H16  | 0.4198| -0.2602| 0.5785| 0.030*| 0.0307| 0.11 |
| C17  | 0.1796 (5)| -0.0909 (3)| 0.5136 (4)| 0.0300 (11)| 0.0307| 0.11 |
| H17  | 0.1374| -0.0196| 0.4938| 0.036*| 0.0307| 0.11 |
| C18  | 0.1090 (5)| -0.1837 (3)| 0.5234 (3)| 0.0312 (11)| 0.0307| 0.11 |
| H18  | 0.0113| -0.1899| 0.5123| 0.037*| 0.0307| 0.11 |
| C19  | 0.1856 (5)| -0.3798 (3)| 0.5707 (3)| 0.0255 (10)| 0.0307| 0.11 |
| Atomic displacement parameters (Å²) |
|-------------------------------------|
|  | $U^{ij}$ |
|  | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
| Fe1 | 0.0196 (5) | 0.0193 (5) | 0.0200 (5) | -0.0042 (4) | -0.0058 (4) | -0.0044 (4) |
| Br1 | 0.0234 (3) | 0.0243 (3) | 0.0308 (3) | 0.0020 (2) | -0.0083 (2) | -0.0093 (2) |
| N1  | 0.022 (2)  | 0.026 (2)  | 0.021 (2)  | 0.0000 (16) | -0.0046 (17) | -0.0062 (16) |
| N2  | 0.031 (2)  | 0.029 (2)  | 0.018 (2)  | -0.0003 (17) | -0.0067 (17) | -0.0041 (16) |
| N3  | 0.018 (2)  | 0.0173 (19)| 0.024 (2)  | -0.0015 (15) | -0.0029 (16) | -0.0046 (15) |
| N4  | 0.021 (2)  | 0.022 (2)  | 0.027 (2)  | -0.0030 (16) | -0.0038 (17) | -0.0052 (16) |
| C1  | 0.031 (3)  | 0.026 (3)  | 0.024 (3)  | 0.001 (2)   | -0.007 (2)   | -0.011 (2)   |
| C2  | 0.037 (3)  | 0.038 (3)  | 0.030 (3)  | 0.007 (2)   | -0.009 (2)   | -0.008 (2)   |
| C3  | 0.044 (3)  | 0.035 (3)  | 0.029 (3)  | 0.012 (2)   | -0.008 (2)   | -0.013 (2)   |
| C4  | 0.038 (3)  | 0.029 (3)  | 0.020 (3)  | 0.005 (2)   | -0.007 (2)   | -0.010 (2)   |
| C5  | 0.038 (3)  | 0.034 (3)  | 0.021 (3)  | 0.000 (2)   | -0.010 (2)   | -0.007 (2)   |
| C6  | 0.042 (3)  | 0.059 (3)  | 0.033 (3)  | 0.007 (3)   | -0.016 (3)   | -0.018 (3)   |
| C7  | 0.062 (4)  | 0.044 (3)  | 0.025 (3)  | 0.016 (3)   | -0.014 (3)   | -0.003 (2)   |
| C8  | 0.055 (4)  | 0.045 (3)  | 0.025 (3)  | 0.002 (3)   | -0.005 (3)   | 0.002 (2)    |
| C9  | 0.035 (3)  | 0.036 (3)  | 0.025 (3)  | 0.003 (2)   | -0.003 (2)   | -0.006 (2)   |
| C10 | 0.044 (3)  | 0.047 (3)  | 0.040 (3)  | -0.011 (3)  | -0.016 (3)   | -0.008 (3)   |
### Geometric parameters (Å, °)

|        |          |          |          |          |          |          |
|--------|----------|----------|----------|----------|----------|----------|
| Fe1—N3 | 2.161 (3) | C12B—H12D | 0.9800   |
| Fe1—N3 | 2.161 (3) | C12B—H12E | 0.9800   |
| Fe1—N1 | 2.190 (3) | C12B—H12F | 0.9800   |
| Fe1—N1 | 2.190 (3) | C13—C14   | 1.528 (7) |
| Fe1—Br1| 2.7040 (5)| C13—C15   | 1.534 (7) |
| Fe1—Br1| 2.7040 (5)| C13—H13   | 1.0000   |
| N1—C1  | 1.300 (5) | C14—H14A  | 0.9800   |
| N1—C2  | 1.377 (5) | C14—H14B  | 0.9800   |
| N2—C1  | 1.354 (5) | C14—H14C  | 0.9800   |
| N2—C3  | 1.360 (5) | C15—H15A  | 0.9800   |
| N2—C4  | 1.442 (5) | C15—H15B  | 0.9800   |
| N3—C16 | 1.309 (5) | C15—H15C  | 0.9800   |
| N3—C17 | 1.370 (5) | C16—H16   | 0.9500   |
| N4—C16 | 1.346 (5) | C17—C18   | 1.359 (6) |
| N4—C18 | 1.373 (5) | C17—H17   | 0.9500   |
| N4—C19 | 1.429 (5) | C18—H18   | 0.9500   |
| C1—H1  | 0.9500   | C19—C24   | 1.397 (6) |
| C2—C3  | 1.369 (6) | C19—C20   | 1.409 (6) |
| C2—H2  | 0.9500   | C20—C21   | 1.381 (6) |
| C3—H3  | 0.9500   | C20—C25   | 1.528 (6) |
| C4—C5  | 1.383 (6) | C21—C22   | 1.381 (7) |
| C4—C9  | 1.393 (6) | C21—H21   | 0.9500   |
| C5—C6  | 1.396 (6) | C22—C23   | 1.371 (6) |

**Table: Crystallographic parameters**

|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
| C11A     | 0.076 (10) | 0.50 (8) | 0.016 (8) | −0.017 (7) | 0.007 (7) |
| C12A     | 0.093 (17) | 0.046 (11) | 0.081 (12) | −0.006 (11) | −0.002 (14) |
| C11B     | 0.14 (2) | 0.065 (11) | 0.060 (15) | −0.045 (13) | 0.042 (13) |
| C12B     | 0.068 (13) | 0.054 (12) | 0.061 (9) | −0.006 (8) | −0.006 (10) |
| C13      | 0.041 (3) | 0.047 (3) | 0.037 (3) | −0.011 (3) | −0.003 (3) |
| C14      | 0.064 (4) | 0.088 (5) | 0.088 (5) | −0.039 (4) | 0.003 (4) |
| C15      | 0.055 (4) | 0.084 (5) | 0.068 (5) | −0.020 (4) | 0.006 (4) |
| C16      | 0.017 (2) | 0.031 (3) | 0.025 (3) | −0.002 (2) | −0.007 (2) |
| C17      | 0.021 (3) | 0.020 (2) | 0.043 (3) | −0.001 (2) | −0.005 (2) |
| C18      | 0.028 (3) | 0.023 (2) | 0.039 (3) | −0.001 (2) | −0.005 (2) |
| C19      | 0.023 (2) | 0.018 (2) | 0.037 (3) | −0.0024 (19) | −0.008 (2) |
| C20      | 0.027 (3) | 0.026 (3) | 0.038 (3) | −0.004 (2) | −0.005 (2) |
| C21      | 0.046 (3) | 0.038 (3) | 0.040 (3) | 0.004 (3) | −0.003 (3) |
| C22      | 0.055 (4) | 0.027 (3) | 0.058 (4) | −0.008 (3) | 0.001 (3) |
| C23      | 0.048 (3) | 0.026 (3) | 0.047 (3) | −0.014 (2) | 0.011 (3) |
| C24      | 0.030 (3) | 0.018 (2) | 0.040 (3) | −0.002 (2) | −0.002 (2) |
| C25      | 0.039 (3) | 0.045 (3) | 0.034 (3) | −0.007 (2) | −0.004 (2) |
| C26      | 0.057 (4) | 0.069 (4) | 0.040 (3) | 0.002 (3) | 0.003 (3) |
| C27      | 0.046 (4) | 0.067 (4) | 0.038 (3) | 0.005 (3) | 0.004 (3) |
| C28      | 0.037 (3) | 0.024 (2) | 0.031 (3) | −0.004 (2) | −0.002 (2) |
| C29      | 0.050 (4) | 0.053 (3) | 0.045 (3) | −0.002 (3) | −0.013 (3) |
| C30      | 0.042 (3) | 0.053 (3) | 0.042 (3) | 0.012 (3) | −0.008 (3) |
### Crystal Structure

| Bond          | Distance | Angle          | Orientation |
|---------------|----------|----------------|-------------|
| C5—C10        | 1.515 (6) |                |             |
| C6—C7         | 1.374 (7) |                |             |
| C6—H6         | 0.950    |                |             |
| C7—C8         | 1.366 (7) |                |             |
| C7—H7         | 0.950    |                |             |
| C8—C9         | 1.384 (6) |                |             |
| C8—H8         | 0.950    |                |             |
| C9—C13        | 1.508 (7) |                |             |
| C10—C12A      | 1.472 (16)|               |             |
| C10—C11B      | 1.492 (17)|               |             |
| C10—C12B      | 1.536 (18)|               |             |
| C10—C11A      | 1.541 (16)|               |             |
| C10—H10A      | 1.000    |                |             |
| C10—H10B      | 1.000    |                |             |
| C11A—H11A     | 0.980    |                |             |
| C11A—H11B     | 0.980    |                |             |
| C11A—H11C     | 0.980    |                |             |
| C12A—H12A     | 0.980    |                |             |
| C12A—H12B     | 0.980    |                |             |
| C12A—H12C     | 0.980    |                |             |
| C11B—H11D     | 0.980    |                |             |
| C11B—H11E     | 0.980    |                |             |
| C11B—H11F     | 0.980    |                |             |

### Bond Angles (deg)

| Bond          | Angle          | Orientation |
|---------------|----------------|-------------|
| N3—Fe1—N3    | 180.0          |             |
| N3—Fe1—N1    | 93.99 (12)     |             |
| N3—Fe1—N1    | 86.01 (12)     |             |
| N3—Fe1—N1    | 86.01 (12)     |             |
| N3—Fe1—N1    | 93.99 (12)     |             |
| N1—Fe1—N1    | 180.0          |             |
| N3—Fe1—Br1   | 90.60 (8)      |             |
| N3—Fe1—Br1   | 89.40 (8)      |             |
| N1—Fe1—Br1   | 89.70 (8)      |             |
| N1—Fe1—Br1   | 90.30 (8)      |             |
| N3—Fe1—Br1   | 89.40 (8)      |             |
| N3—Fe1—Br1   | 90.60 (8)      |             |
| N1—Fe1—Br1   | 90.30 (8)      |             |
| N1—Fe1—Br1   | 89.70 (8)      |             |
| C1—N1—C2     | 105.3 (3)      |             |
| C1—N1—Fe1    | 124.7 (3)      |             |
| C2—N1—Fe1    | 129.8 (3)      |             |
| C1—N2—C3     | 106.8 (4)      |             |
| C1—N2—C4     | 125.9 (3)      |             |
| C3—N2—C4     | 127.2 (4)      |             |
| C16—N3—C17   | 104.8 (3)      |             |
| C16—N3—Fe1   | 127.3 (3)      |             |
| C17—N3—Fe1   | 126.0 (3)      |             |

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| Bond/Centers | Distance (Å) | Bond/Centers | Distance (Å) |
|-------------|-------------|-------------|-------------|
| C16—N4—C18 | 107.1 (3)   | N4—C16—H16 | 123.9       |
| C16—N4—C19 | 127.6 (3)   | C18—C17—N3 | 110.8 (4)   |
| C18—N4—C19 | 125.3 (4)   | C18—C17—H17| 124.6       |
| N1—C1—N2   | 112.4 (4)   | N3—C17—H17 | 124.6       |
| N1—C1—H1   | 123.8       | C17—C18—N4 | 105.1 (4)   |
| N2—C1—H1   | 123.8       | C17—C18—H18| 127.5       |
| C3—C2—N1   | 109.5 (4)   | N4—C18—H18 | 127.5       |
| C3—C2—H2   | 125.3       | C24—C19—C20| 122.3 (4)   |
| N1—C2—H2   | 125.3       | C24—C19—N4 | 118.7 (4)   |
| N2—C3—C2   | 106.0 (4)   | C20—C19—N4 | 118.9 (4)   |
| N2—C3—H3   | 127.0       | C21—C20—C19| 117.2 (4)   |
| C2—C3—H3   | 127.0       | C21—C20—C25| 121.7 (4)   |
| C5—C4—C9   | 123.8 (4)   | C19—C20—C25| 121.1 (4)   |
| C5—C4—N2   | 118.2 (4)   | C20—C21—C22| 121.2 (4)   |
| C9—C4—N2   | 118.0 (4)   | C20—C21—H21| 119.4       |
| C4—C5—C6   | 117.1 (4)   | C22—C21—H21| 119.4       |
| C4—C5—C10  | 122.5 (4)   | C23—C22—C21| 120.0 (5)   |
| C6—C5—C10  | 120.3 (5)   | C23—C22—H22| 120.0       |
| C7—C6—C5   | 120.4 (5)   | C21—C22—H22| 120.0       |
| C7—C6—H6   | 119.8       | C22—C23—C24| 121.9 (5)   |
| C5—C6—H6   | 119.8       | C22—C23—H23| 119.1       |
| C8—C7—C6   | 120.5 (5)   | C24—C23—H23| 119.1       |
| C8—C7—H7   | 119.7       | C23—C24—C19| 117.3 (4)   |
| C6—C7—H7   | 119.7       | C23—C24—C28| 120.8 (4)   |
| C7—C8—C9   | 122.0 (5)   | C19—C24—C28| 121.9 (4)   |
| C7—C8—H8   | 119.0       | C26—C25—C27| 110.5 (4)   |
| C9—C8—H8   | 119.0       | C26—C25—C20| 111.9 (4)   |
| C8—C9—C4   | 116.1 (5)   | C27—C25—C20| 112.3 (4)   |
| C4—C9—C13  | 122.5 (5)   | C26—C25—H25| 107.3       |
| C12A—C10—C5| 121.4 (4)   | C27—C25—H25| 107.3       |
| C12B—C10—C5| 121.4 (10)  | C20—C25—H25| 107.3       |
| C11B—C10—C5| 108.1 (10)  | C25—C26—H26A| 109.5       |
| C11B—C10—C12B| 86.9 (11)| C25—C26—H26B| 109.5       |
| C5—C10—C12B| 113.7 (10)  | H26A—C26—H26B| 109.5       |
| C12A—C10—C11A| 129.6 (13)| C25—C26—H26C| 109.5       |
| C5—C10—C11A| 112.4 (9)   | H26A—C26—H26C| 109.5       |
| C12A—C10—H10A| 97.7         | H26B—C26—H26C| 109.5       |
| C5—C10—H10A| 97.7         | C25—C27—H27C| 109.5       |
| C11A—C10—H10A| 97.7        | C25—C27—H27B| 109.5       |
| C11B—C10—H10B| 115.0       | H27C—C27—H27B| 109.5       |
| C5—C10—H10B| 115.0       | C25—C27—H27A| 109.5       |
| C12B—C10—H10B| 115.0       | H27C—C27—H27A| 109.5       |
| C10—C11A—H11A| 109.5       | H27B—C27—H27A| 109.5       |
| C10—C11A—H11B| 109.5       | C30—C28—C29| 110.3 (4)   |
| H11A—C11A—H11B| 109.5     | C30—C28—C24| 110.4 (4)   |
| C10—C11A—H11C| 109.5       | C29—C28—C24| 112.0 (4)   |
| H11A—C11A—H11C| 109.5       | C30—C28—H28| 108.0       |
| H11B—C11A—H11C| 109.5       | C29—C28—H28| 108.0       |
C10—C12A—H12A 109.5
C10—C12A—H12B 109.5
H12A—C12A—H12B 109.5
C10—C12A—H12C 109.5
H12A—C12A—H12C 109.5
H12B—C12A—H12C 109.5
C10—C11B—H11D 109.5
C10—C11B—H11E 109.5
H11D—C11B—H11E 109.5
C10—C11B—H11F 109.5
H11D—C11B—H11F 109.5
H11E—C11B—H11F 109.5
C10—C12B—H12D 109.5
C10—C12B—H12E 109.5
C2—N1—C1—N2 −0.1 (5)
Fe1—N1—C1—N2 −175.1 (3)
C3—N2—C1—N1 0.1 (5)
C4—N2—C1—N1 −176.3 (4)
C1—N1—C2—C3 0.0 (5)
Fe1—N1—C2—C3 174.7 (3)
C1—N2—C3—C2 −0.1 (5)
C4—N2—C3—C2 176.2 (4)
N1—C2—C3—N2 0.0 (6)
C1—N2—C3—C2 −94.1 (5)
C3—N2—C4—C5 90.3 (6)
C1—N2—C4—C5 83.6 (6)
C3—N2—C4—C5 −92.0 (5)
C9—C4—C5—C6 2.8 (7)
C9—C4—C5—C6 −175.2 (4)
N2—C4—C5—C6 −179.7 (4)
C9—C4—C5—C10 2.3 (6)
N2—C4—C5—C10 −175.2 (4)
C4—C5—C6—C7 −0.2 (6)
C4—C5—C6—C7 177.8 (4)
C5—C6—C7—C8 −1.8 (7)
C6—C7—C8—C9 1.4 (8)
C7—C8—C9—C4 1.0 (7)
C7—C8—C9—C13 −176.9 (5)
C5—C4—C9—C8 −3.1 (7)
N2—C4—C9—C8 179.4 (4)
C5—C4—C9—C13 174.7 (4)
N2—C4—C9—C13 −2.8 (6)
C4—C5—C10—C12A −112.3 (9)
C6—C5—C10—C12A 69.8 (9)
C4—C5—C10—C11B 122.2 (9)
C6—C5—C10—C11B −55.7 (10)
C4—C5—C10—C12B −143.2 (7)
C6—C5—C10—C12B 39.0 (8)
C24—C28—H28 108.0
C28—C29—H29A 109.5
C28—C29—H29B 109.5
H29A—C29—H29B 109.5
C28—C29—H29C 109.5
H29A—C29—H29C 109.5
C28—C29—H29C 109.5
H29B—C29—H29C 109.5
C28—C30—H30C 109.5
C28—C30—H30B 109.5
H30C—C30—H30B 109.5
C28—C30—H30A 109.5
H30C—C30—H30A 109.5
C28—C30—H30A 109.5
C8—C9—C13—C15 −38.0 (7)
C4—C9—C13—C15 144.3 (5)
C17—N3—C16—N4 −0.1 (5)
Fe1—N3—C16—N4 −164.9 (3)
C19—N4—C16—N3 0.0 (5)
Fe1—N4—C16—N3 178.8 (4)
C16—N3—C17—C18 0.1 (5)
Fe1—N3—C17—C18 165.2 (3)
N3—C17—C18—N4 −0.1 (5)
C16—N4—C18—C17 0.1 (4)
C19—N4—C18—C17 −178.7 (4)
C16—N4—C19—C24 100.9 (5)
C18—N4—C19—C24 −80.5 (5)
C19—N4—C19—C20 100.9 (5)
C16—N4—C19—C20 −77.7 (6)
C18—N4—C19—C20 100.9 (5)
C16—N4—C19—C21 3.6 (7)
N4—C19—C20—C21 −177.9 (4)
C24—C19—C20—C25 −176.6 (4)
C4—C19—C20—C25 1.9 (6)
C19—C20—C21—C22 −1.8 (7)
C25—C20—C21—C22 178.4 (5)
C20—C21—C22—C23 0.1 (8)
C21—C22—C23—C24 0.0 (8)
C22—C23—C24—C19 1.7 (8)
C22—C23—C24—C28 179.8 (5)
C20—C19—C24—C23 −3.5 (7)
N4—C19—C24—C23 177.9 (4)
C20—C19—C24—C28 178.3 (4)
N4—C19—C24—C28 −0.2 (6)
C21—C20—C25—C26 103.5 (5)
C19—C20—C25—C26 −76.2 (6)
C21—C20—C25—C27 −21.4 (7)
C19—C20—C25—C27 158.8 (4)
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supporting information

C4—C5—C10—C11A  91.2 (8)  C23—C24—C28—C30  −74.1 (6)
C6—C5—C10—C11A  −86.7 (8)  C19—C24—C28—C30  104.0 (5)
C8—C9—C13—C14  86.1 (6)  C23—C24—C28—C29  49.2 (6)
C4—C9—C13—C14  −91.6 (6)  C19—C24—C28—C29 −132.7 (5)

Symmetry code: (i) −x+1, −y, −z+1.

Hydrogen-bond geometry (Å, °)
Cg3 and Cg4 are the centroids of rings C4–C9 and C19–C24, respectively.

\[ \begin{array}{cccc}
D—H···A & D—H & H···A & D···A \\
C1—H1···Br1^i & 0.95 & 2.71 & 3.368 (4) & 127 \\
C2—H2···Br1 & 0.95 & 2.91 & 3.477 (5) & 119 \\
C16—H16···Br1 & 0.95 & 2.81 & 3.373 (4) & 119 \\
C17—H17···Br1^i & 0.95 & 2.91 & 3.484 (4) & 120 \\
C18—H18···Br1^ii & 0.95 & 2.77 & 3.707 (5) & 167 \\
C27—H27A···Cg4^iii & 0.98 & 2.92 & 3.639 (6) & 131 \\
C30—H30C···Cg3^iv & 0.98 & 2.88 & 3.862 (6) & 177 \\
\end{array} \]

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

(IIb) trans-Dibromidotetrakis[1-(2,6-diisopropylphenyl)-1H-imidazole-κN^3]iron(II) diethyl ether disolvate

Crystal data
[FeBr₂(C₁₅H₂₀N₂)₄]·₂C₄H₁₀O

\[ Z = 1 \]
\[ F(000) = 676 \]

Triclinic, \( P \)

\[ a = 11.6710 (8) \text{ Å} \]
\[ b = 12.4758 (9) \text{ Å} \]
\[ c = 13.5759 (10) \text{ Å} \]
\[ α = 64.464 (5)° \]
\[ β = 81.515 (6)° \]
\[ γ = 88.982 (6)° \]

\[ V = 1761.8 (2) \text{ Å}^³ \]

Data collection

Stoe IPDS 2
diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
\( ϕ + ω \) scans
Absorption correction: multi-scan
(MULscanABS in PLATON; Spek, 2009)
\( T_{\text{min}} = 0.557, T_{\text{max}} = 0.672 \)

Refinement

Refinement on \( F^2 \)
Least-squares matrix: full
\( R[F^2 > 2σ(F^2)] = 0.031 \)
\( wR(F^2) = 0.077 \)
\( S = 1.03 \)
6374 reflections
378 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
supporting information

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

\[ \Delta \rho_{\text{max}} = 0.44 \text{ e Å}^{-3} \]

\[ \Delta \rho_{\text{min}} = -0.37 \text{ e Å}^{-3} \]

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

| Atom | x    | y    | z    | Uiso/Ueq | Occ. (<1) |
|------|------|------|------|----------|-----------|
| Fe1  | 0.5000 | 1.0000 | 0.5000 | 0.02343 (9) |
| Br1  | 0.37430 (2) | 0.79434 (2) | 0.64396 (2) | 0.02939 (7) |
| N1   | 0.46601 (13) | 1.07022 (14) | 0.62346 (13) | 0.0270 (3) |
| N2   | 0.48075 (14) | 1.18785 (14) | 0.70489 (13) | 0.0278 (3) |
| N3   | 0.65641 (13) | 0.93155 (14) | 0.57112 (13) | 0.0271 (3) |
| N4   | 0.75321 (13) | 0.80847 (14) | 0.69892 (13) | 0.0277 (3) |
| C1   | 0.50151 (17) | 1.17670 (17) | 0.60955 (16) | 0.0285 (4) |
| H1   | 0.5371 | 1.2375 | 0.5410 | 0.034* |
| C2   | 0.42078 (17) | 1.01038 (18) | 0.73346 (17) | 0.0315 (4) |
| H2   | 0.3885 | 0.9310 | 0.7684 | 0.038* |
| C3   | 0.42911 (18) | 1.08153 (18) | 0.78454 (17) | 0.0330 (4) |
| H3   | 0.4042 | 1.0619 | 0.8604 | 0.040* |
| C4   | 0.51202 (18) | 1.29018 (17) | 0.72041 (16) | 0.0293 (4) |
| C5   | 0.61769 (19) | 1.29155 (18) | 0.75702 (17) | 0.0344 (4) |
| C6   | 0.6449 (2) | 1.3901 (2) | 0.77407 (19) | 0.0437 (5) |
| H6   | 0.7154 | 1.3940 | 0.7998 | 0.052* |
| C7   | 0.5708 (3) | 1.4816 (2) | 0.75409 (19) | 0.0491 (6) |
| H7   | 0.5910 | 1.5477 | 0.7664 | 0.059* |
| C8   | 0.4679 (2) | 1.47935 (19) | 0.71658 (19) | 0.0462 (6) |
| H8   | 0.4186 | 1.5440 | 0.7027 | 0.055* |
| C9   | 0.43549 (19) | 1.38246 (18) | 0.69876 (17) | 0.0355 (5) |
| C10  | 0.7014 (2) | 1.1920 (2) | 0.7763 (2) | 0.0439 (5) |
| H10  | 0.6593 | 1.1250 | 0.7725 | 0.053* |
| C11  | 0.8047 (3) | 1.2317 (3) | 0.6846 (3) | 0.0823 (11) |
| H11A | 0.8487 | 1.2969 | 0.6861 | 0.099* |
| H11B | 0.7776 | 1.2589 | 0.6131 | 0.099* |
| H11C | 0.8547 | 1.1648 | 0.6952 | 0.099* |
| C12  | 0.7368 (4) | 1.1444 (4) | 0.8904 (3) | 0.0943 (13) |
| H12C | 0.7884 | 1.0789 | 0.9003 | 0.113* |
| H12B | 0.6674 | 1.1154 | 0.9467 | 0.113* |
| H12A | 0.7773 | 1.2081 | 0.8976 | 0.113* |
| C13  | 0.3209 (2) | 1.3778 (2) | 0.6609 (2) | 0.0454 (5) |
| H13  | 0.3215 | 1.3104 | 0.6396 | 0.054* |
| C14  | 0.2197 (3) | 1.3530 (3) | 0.7540 (3) | 0.0751 (10) |
| H14A | 0.2156 | 1.4191 | 0.7751 | 0.090* |
| H14B | 0.2313 | 1.2792 | 0.8180 | 0.090* |
| Atom | x       | y       | z       | Ueq     |
|------|---------|---------|---------|---------|
| H14C | 0.1472  | 1.3448  | 0.7290  | 0.090*  |
| C15  | 0.3026 (3) | 1.4921 (3) | 0.5592 (2) | 0.0691 (8) |
| H15A | 0.3672  | 1.5066  | 0.4992  | 0.083*  |
| H15B | 0.2992  | 1.5595  | 0.5784  | 0.083*  |
| H15C | 0.2297  | 1.4831  | 0.5351  | 0.083*  |
| C16  | 0.66540 (16) | 0.82018 (17) | 0.64133 (16) | 0.0271 (4) |
| H16  | 0.6160  | 0.7559  | 0.6503  | 0.033*  |
| C17  | 0.74340 (17) | 0.99506 (18) | 0.58507 (18) | 0.0339 (4) |
| H17  | 0.7588  | 1.0786  | 0.5454  | 0.041*  |
| C18  | 0.80359 (17) | 0.92076 (18) | 0.66367 (18) | 0.0347 (5) |
| H18  | 0.8673  | 0.9417  | 0.6892  | 0.042*  |
| C19  | 0.77470 (17) | 0.70242 (18) | 0.79383 (18) | 0.0336 (4) |
| H20  | 0.7010 (2) | 0.67551 (19) | 0.89322 (19) | 0.0395 (5) |
| C20  | 0.7219 (3) | 0.5728 (2) | 0.9846 (2) | 0.0537 (6) |
| H21  | 0.6734  | 0.5507  | 1.0537  | 0.064*  |
| C22  | 0.8125 (3) | 0.5027 (2) | 0.9759 (3) | 0.0635 (8) |
| H22  | 0.8257  | 0.4336  | 1.0392  | 0.076*  |
| C23  | 0.8837 (2) | 0.5320 (2) | 0.8765 (3) | 0.0563 (7) |
| H23  | 0.9452  | 0.4826  | 0.8722  | 0.068*  |
| C24  | 0.86670 (18) | 0.6333 (2) | 0.7823 (2) | 0.0417 (5) |
| C25  | 0.6018 (2) | 0.7531 (2) | 0.90310 (19) | 0.0436 (5) |
| H25  | 0.6034  | 0.8222  | 0.8292  | 0.052*  |
| C26  | 0.6170 (3) | 0.8022 (3) | 0.9863 (2) | 0.0613 (7) |
| H26A | 0.6150  | 0.7362  | 1.0598  | 0.074*  |
| H26B | 0.5540  | 0.8546  | 0.9883  | 0.074*  |
| H26C | 0.6916  | 0.8474  | 0.9640  | 0.074*  |
| C27  | 0.4846 (2) | 0.6854 (2) | 0.9333 (2) | 0.0513 (6) |
| H27C | 0.4228  | 0.7357  | 0.9430  | 0.062*  |
| H27B | 0.4834  | 0.6129  | 1.0023  | 0.062*  |
| H27A | 0.4724  | 0.6639  | 0.8740  | 0.062*  |
| C28  | 0.9445 (2) | 0.6657 (2) | 0.6726 (2) | 0.0525 (7) |
| H28  | 0.9153  | 0.7391  | 0.6165  | 0.063*  |
| C29  | 0.9413 (3) | 0.5689 (3) | 0.6332 (3) | 0.0709 (8) |
| H29A | 0.9677  | 0.4951  | 0.6878  | 0.085*  |
| H29B | 0.9924  | 0.5936  | 0.5623  | 0.085*  |
| H29C | 0.8618  | 0.5555  | 0.6243  | 0.085*  |
| C30  | 1.0691 (3) | 0.6943 (4) | 0.6787 (4) | 0.0895 (12) |
| H30C | 1.1168  | 0.7180  | 0.6062  | 0.107*  |
| H30B | 1.1001  | 0.6237  | 0.7334  | 0.107*  |
| H30A | 1.0706  | 0.7595  | 0.7006  | 0.107*  |
| O1   | 0.96877 (19) | 1.0413 (2) | 0.2300 (2) | 0.0818 (7) |
| C31  | 0.9192 (4) | 1.1111 (4) | 0.1369 (4) | 0.1043 (14) |
| H31A | 0.8628  | 1.1632  | 0.1541  | 0.125*  |
| H31B | 0.8777  | 1.0599  | 0.1133  | 0.125*  |
| C32  | 1.0118 (4) | 1.1834 (5) | 0.0486 (4) | 0.1199 (18) |
| H32A | 1.0544  | 1.2315  | 0.0737  | 0.180*  |
| H32B | 0.9780  | 1.2359  | −0.0165 | 0.180*  |
| H32C | 1.0650  | 1.1313  | 0.0294  | 0.180*  |
|       | U_{11}  | U_{22}  | U_{33}  | U_{12}  | U_{13}  | U_{23}  |
|-------|---------|---------|---------|---------|---------|---------|
| Fe1   | 0.02406 (18) | 0.01970 (18) | 0.0303 (2) | 0.00385 (13) | −0.00785 (14) | −0.01329 (16) |
| Br1   | 0.02990 (11) | 0.02252 (10) | 0.03696 (12) | 0.00061 (7) | −0.00611 (7) | −0.01369 (8) |
| N1    | 0.0280 (8) | 0.0245 (8) | 0.0330 (9) | 0.0040 (6) | −0.0080 (6) | −0.0156 (7) |
| N2    | 0.0342 (8) | 0.0222 (8) | 0.0294 (8) | 0.0015 (6) | −0.0043 (7) | −0.0135 (7) |
| N3    | 0.0247 (8) | 0.0249 (8) | 0.0330 (9) | 0.0024 (6) | −0.0068 (6) | −0.0132 (7) |
| N4    | 0.0250 (8) | 0.0253 (8) | 0.0329 (9) | 0.0037 (6) | −0.0086 (6) | −0.0115 (7) |
| C1    | 0.0331 (10) | 0.0238 (9) | 0.0314 (10) | 0.0026 (7) | −0.0039 (8) | −0.0149 (8) |
| C2    | 0.0347 (10) | 0.0243 (10) | 0.0351 (11) | −0.0027 (8) | −0.0043 (8) | −0.0125 (8) |
| C3    | 0.0412 (11) | 0.0268 (10) | 0.0301 (10) | −0.0038 (8) | −0.0016 (8) | −0.0125 (9) |
| C4    | 0.0423 (11) | 0.0216 (9) | 0.0262 (10) | −0.0019 (8) | −0.0006 (8) | −0.0135 (8) |
| C5    | 0.0438 (11) | 0.0286 (10) | 0.0300 (10) | −0.0056 (9) | −0.0018 (9) | −0.0128 (9) |
| C6    | 0.0598 (14) | 0.0357 (12) | 0.0372 (12) | −0.0131 (10) | −0.0058 (10) | −0.0173 (10) |
| C7    | 0.0852 (19) | 0.0279 (11) | 0.0364 (12) | −0.0125 (11) | −0.0013 (12) | −0.0179 (10) |
| C8    | 0.0772 (17) | 0.0226 (10) | 0.0358 (12) | 0.0077 (10) | 0.0014 (11) | −0.0133 (9) |
| C9    | 0.0493 (12) | 0.0251 (10) | 0.0288 (10) | 0.0055 (9) | 0.0004 (9) | −0.0109 (9) |
| C10   | 0.0427 (12) | 0.0370 (12) | 0.0562 (14) | 0.0005 (10) | −0.0146 (11) | −0.0219 (11) |
| C11   | 0.0598 (18) | 0.062 (2) | 0.117 (3) | 0.0044 (15) | 0.0155 (18) | −0.040 (2) |
| C12   | 0.121 (3) | 0.090 (3) | 0.086 (3) | 0.050 (2) | −0.059 (2) | −0.039 (2) |
| C13   | 0.0495 (13) | 0.0399 (13) | 0.0452 (13) | 0.0150 (10) | −0.0078 (10) | −0.0173 (11) |
| C14   | 0.0509 (16) | 0.098 (3) | 0.0563 (17) | 0.0181 (16) | −0.0052 (13) | −0.0164 (17) |
| C15   | 0.082 (2) | 0.068 (2) | 0.0461 (16) | 0.0163 (16) | −0.0181 (14) | −0.0116 (14) |
| C16   | 0.0258 (9) | 0.0245 (9) | 0.0340 (10) | 0.0034 (7) | −0.0076 (7) | −0.0145 (8) |
| C17   | 0.0312 (10) | 0.0255 (10) | 0.0435 (12) | −0.0023 (8) | −0.0101 (9) | −0.0119 (9) |
| C18   | 0.0289 (10) | 0.0306 (11) | 0.0454 (12) | −0.0002 (8) | −0.0137 (9) | −0.0146 (9) |
| C19   | 0.0340 (10) | 0.0260 (10) | 0.0394 (11) | 0.0025 (8) | −0.0165 (9) | −0.0095 (9) |
| C20   | 0.0491 (13) | 0.0320 (11) | 0.0372 (12) | 0.0002 (9) | −0.0137 (10) | −0.0124 (10) |
| C21   | 0.0744 (18) | 0.0425 (14) | 0.0386 (13) | 0.0002 (12) | −0.0210 (12) | −0.0084 (11) |
| C22   | 0.081 (2) | 0.0366 (14) | 0.0631 (18) | 0.0086 (13) | −0.0413 (16) | −0.0030 (13) |
| C23   | 0.0499 (14) | 0.0365 (13) | 0.078 (2) | 0.0128 (11) | −0.0308 (14) | −0.0146 (13) |
| C24   | 0.0311 (11) | 0.0319 (11) | 0.0608 (15) | 0.0057 (9) | −0.0182 (10) | −0.0155 (11) |
### Geometric parameters (Å, °)

|                  |                  |                  |                  |                  |                  |                  |
|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| **Fe1—N3**       | 2.1789 (15)      | **C18—H18**     |                  |                  |                  | 0.9500           |
| **Fe1—N3**       | 2.1789 (15)      | **C19—C20**     |                  |                  |                  | 1.397 (3)        |
| **Fe1—N1**       | 2.1889 (16)      | **C19—C24**     |                  |                  |                  | 1.399 (3)        |
| **Fe1—N1**       | 2.1889 (16)      | **C20—C21**     |                  |                  |                  | 1.396 (3)        |
| **Fe1—Br1**      | 2.7422 (3)       | **C20—C25**     |                  |                  |                  | 1.523 (3)        |
| **Fe1—Br1**      | 2.7422 (3)       | **C21—C22**     |                  |                  |                  | 1.384 (4)        |
| **N1—C1**        | 1.324 (2)        | **C21—H21**     |                  |                  |                  | 0.9500           |
| **N1—C2**        | 1.373 (3)        | **C22—C23**     |                  |                  |                  | 1.378 (4)        |
| **N2—C1**        | 1.347 (2)        | **C22—H22**     |                  |                  |                  | 0.9500           |
| **N2—C3**        | 1.375 (3)        | **C23—C24**     |                  |                  |                  | 1.395 (3)        |
| **N2—C4**        | 1.442 (2)        | **C23—H23**     |                  |                  |                  | 0.9500           |
| **N3—C16**       | 1.316 (2)        | **C24—C28**     |                  |                  |                  | 1.516 (4)        |
| **N3—C17**       | 1.382 (2)        | **C25—C27**     |                  |                  |                  | 1.527 (4)        |
| **N4—C16**       | 1.347 (2)        | **C25—C26**     |                  |                  |                  | 1.530 (3)        |
| **N4—C18**       | 1.380 (3)        | **C25—H25**     |                  |                  |                  | 1.0000           |
| **N4—C19**       | 1.445 (3)        | **C26—H26A**    |                  |                  |                  | 0.9800           |
| **C1—H1**        | 0.9500           | **C26—H26B**    |                  |                  |                  | 0.9800           |
| **C2—C3**        | 1.354 (3)        | **C26—H26C**    |                  |                  |                  | 0.9800           |
| **C2—H2**        | 0.9500           | **C27—H27C**    |                  |                  |                  | 0.9800           |
| **C3—H3**        | 0.9500           | **C27—H27B**    |                  |                  |                  | 0.9800           |
| **C4—C5**        | 1.399 (3)        | **C27—H27A**    |                  |                  |                  | 0.9800           |
| **C4—C9**        | 1.400 (3)        | **C28—C29**     |                  |                  |                  | 1.521 (4)        |
| **C5—C6**        | 1.395 (3)        | **C28—C30**     |                  |                  |                  | 1.526 (4)        |
| **C5—C10**       | 1.522 (3)        | **C28—H28**     |                  |                  |                  | 1.0000           |
| **C6—C7**        | 1.376 (4)        | **C29—H29A**    |                  |                  |                  | 0.9800           |
| **C6—H6**        | 0.9500           | **C29—H29B**    |                  |                  |                  | 0.9800           |
| **C7—C8**        | 1.376 (4)        | **C29—H29C**    |                  |                  |                  | 0.9800           |
| **C7—H7**        | 0.9500           | **C30—H30C**    |                  |                  |                  | 0.9800           |
| **C8—C9**        | 1.399 (3)        | **C30—H30B**    |                  |                  |                  | 0.9800           |
| **C8—H8**        | 0.9500           | **C30—H30A**    |                  |                  |                  | 0.9800           |
| **C9—C13**       | 1.512 (3)        | **O1—C31**      |                  |                  |                  | 1.393 (5)        |
| **C10—C11**      | 1.516 (4)        | **O1—C33B**     |                  |                  |                  | 1.416 (9)        |
| Bond                  | Distance   | Bond                  | Distance   |
|----------------------|------------|----------------------|------------|
| C10—C12              | 1.519 (4)  | O1—C33A              | 1.539 (9)  |
| C10—H10              | 1.0000     | C31—C32              | 1.462 (6)  |
| C11—H11A             | 0.9800     | C31—H31A             | 0.9900     |
| C11—H11B             | 0.9800     | C31—H31B             | 0.9900     |
| C11—H11C             | 0.9800     | C32—H32A             | 0.9800     |
| C12—H12C             | 0.9800     | C32—H32B             | 0.9800     |
| C12—H12B             | 0.9800     | C32—H32C             | 0.9800     |
| C12—H12A             | 0.9800     | C33A—C34A            | 1.473 (14) |
| C13—C14              | 1.525 (4)  | C33A—H33A            | 0.9900     |
| C13—C15              | 1.538 (4)  | C33A—H33B            | 0.9900     |
| C13—H13              | 1.0000     | C33B—C34B            | 1.433 (14) |
| C14—H14A             | 0.9800     | C33B—H33D            | 0.9900     |
| C14—H14B             | 0.9800     | C33B—H33E            | 0.9900     |
| C14—H14C             | 0.9800     | C34A—H34A            | 0.9800     |
| C15—H15A             | 0.9800     | C34A—H34B            | 0.9800     |
| C15—H15B             | 0.9800     | C34A—H34C            | 0.9800     |
| C15—H15C             | 0.9800     | C34B—H34D            | 0.9800     |
| C16—H16              | 0.9500     | C34B—H34E            | 0.9800     |
| C17—C18              | 1.355 (3)  | C34B—H34F            | 0.9800     |
| C17—H17              | 0.9500     |                      |            |

N3—Fe1—N3  180.00 (3)  C17—C18—N4  105.81 (17)
N3—Fe1—N1  93.88 (6)   C17—C18—H18  127.1
N3—Fe1—N1' 86.12 (6)   N4—C18—H18  127.1
N3—Fe1—N1'' 86.12 (6)  C20—C19—C24  123.7 (2)
N3—Fe1—N1'' 93.88 (6)  C20—C19—N4  116.99 (18)
N1—Fe1—N1' 180.00 (6)  C24—C19—N4  119.3 (2)
N3—Fe1—Br1  88.74 (4)  C21—C20—C24  116.8 (2)
N3—Fe1—Br1' 91.26 (4)  C21—C20—C25  120.8 (2)
N1—Fe1—Br1  89.88 (4)  C19—C20—C25  122.40 (19)
N1—Fe1—Br1' 90.12 (4)  C22—C21—C20  120.9 (3)
N3—Fe1—Br1' 91.26 (4)  C22—C21—H21  119.6
N3—Fe1—Br1' 88.74 (4)  C20—C21—H21  119.6
N1—Fe1—Br1' 90.12 (4)  C23—C22—C21  120.8 (2)
N1—Fe1—Br1' 89.88 (4)  C23—C22—H22  119.6
Br1—Fe1—Br1' 180.0  C21—C22—H22  119.6
C1—N1—C2  105.58 (16)  C22—C23—C24  120.9 (2)
C1—N1—Fe1  125.49 (13)  C22—C23—H23  119.6
C2—N1—Fe1  128.27 (13)  C24—C23—H23  119.6
C1—N2—C3  106.83 (16)  C23—C24—C19  116.9 (2)
C1—N2—C4  126.10 (16)  C23—C24—C28  121.1 (2)
C3—N2—C4  127.01 (16)  C19—C24—C28  122.0 (2)
C16—N3—C17 105.29 (16)  C20—C25—C27  111.2 (2)
C16—N3—Fe1 123.77 (12)  C20—C25—C26  111.3 (2)
C17—N3—Fe1 127.33 (13)  C27—C25—C26  110.9 (2)
C16—N4—C18 107.06 (16)  C20—C25—H25  107.7
C16—N4—C19 125.48 (16)  C27—C25—H25  107.7
C18—N4—C19 126.45 (16)  C26—C25—H25  107.7
| Bond                  | Distance (Å) | Angle (°)  |
|----------------------|--------------|------------|
| N1—C1—N2            | 111.41 (17)  |            |
| N1—C1—H1            | 124.3        |            |
| N2—C1—H1            | 124.3        |            |
| C3—C2—N1            | 109.73 (17)  |            |
| C3—C2—H2            | 125.1        |            |
| N1—C2—H2            | 125.1        |            |
| C2—C3—N2            | 106.44 (18)  |            |
| C2—C3—H3            | 126.8        |            |
| N2—C3—H3            | 126.8        |            |
| C5—C4—C9            | 123.38 (18)  |            |
| C5—C4—N2            | 117.93 (17)  |            |
| C9—C4—N2            | 118.68 (18)  |            |
| C6—C5—C4            | 117.0 (2)    |            |
| C6—C5—C10           | 120.6 (2)    |            |
| C4—C5—C10           | 122.40 (18)  |            |
| C7—C6—C5            | 120.8 (2)    |            |
| C7—C6—H6            | 119.6        |            |
| C5—C6—H6            | 119.6        |            |
| C6—C7—C8            | 121.4 (2)    |            |
| C6—C7—H7            | 119.3        |            |
| C8—C7—H7            | 119.3        |            |
| C7—C8—C9            | 120.5 (2)    |            |
| C7—C8—H8            | 119.8        |            |
| C9—C8—H8            | 119.8        |            |
| C8—C9—C4            | 117.0 (2)    |            |
| C8—C9—C13           | 120.7 (2)    |            |
| C4—C9—C13           | 122.26 (19)  |            |
| C11—C10—C12         | 112.6 (3)    |            |
| C11—C10—C5          | 110.5 (2)    |            |
| C12—C10—C5          | 112.1 (2)    |            |
| C11—C10—H10         | 107.1        |            |
| C12—C10—H10         | 107.1        |            |
| C5—C10—H10          | 107.1        |            |
| C10—C11—H11A        | 109.5        |            |
| C10—C11—H11B        | 109.5        |            |
| H11A—C11—H11B       | 109.5        |            |
| C10—C11—H11C        | 109.5        |            |
| H11A—C11—H11C       | 109.5        |            |
| H11B—C11—H11C       | 109.5        |            |
| C10—C12—H12C        | 109.5        |            |
| C10—C12—H12B        | 109.5        |            |
| H12C—C12—H12B       | 109.5        |            |
| C10—C12—H12A        | 109.5        |            |
| H12C—C12—H12A       | 109.5        |            |
| C9—C13—C14          | 111.1 (2)    |            |
| C9—C13—C15          | 112.4 (2)    |            |
| C14—C13—C15         | 110.0 (2)    |            |
| Bond                  | Distance | Angles                           | Error |
|-----------------------|----------|----------------------------------|-------|
| C9—C13—H13           | 107.7    | O1—C33A—H33B                    | 110.3 |
| C14—C13—H13          | 107.7    | H33A—C33A—H33B                  | 108.5 |
| C15—C13—H13          | 107.7    | O1—C33B—C34B                    | 108.2 |
| C13—C14—H14A         | 109.5    | O1—C33B—H33D                    | 110.1 |
| C13—C14—H14B         | 109.5    | C34B—C33B—H33D                  | 110.1 |
| H14A—C14—H14B        | 109.5    | O1—C33B—H33E                    | 110.1 |
| C13—C14—H14C         | 109.5    | C34B—C33B—H33E                  | 110.1 |
| H14A—C14—H14C        | 109.5    | H33D—C33B—H33E                  | 108.4 |
| H14B—C14—H14C        | 109.5    | C33A—C34A—H34A                  | 109.5 |
| C13—C15—H15A         | 109.5    | C33A—C34A—H34B                  | 109.5 |
| C13—C15—H15B         | 109.5    | H34A—C34A—H34B                  | 109.5 |
| H15A—C15—H15B        | 109.5    | C33A—C34A—H34C                  | 109.5 |
| C13—C15—H15C         | 109.5    | H34A—C34A—H34C                  | 109.5 |
| H15A—C15—H15C        | 109.5    | H34B—C34A—H34C                  | 109.5 |
| C3—N1—C1—C2          | 177.60   | C33B—C34B—H34D                  | 109.5 |
| C4—N2—C1—C3          | 0.2 (2)  | N3—C17—C18—N4                   | 0.3 (2) |
| C1—N1—C2—C3          | 0.2 (2)  | C16—N4—C18—C17                  | −0.5 (2) |
| Fe1—N1—C2—C3         | 171.21 (14) | C19—N4—C18—C17             | −169.40 (19) |
| N1—C2—C3—N2          | −0.1 (2) | C16—N4—C19—C20                 | −74.2 (3) |
| C1—N2—C3—C2          | −0.1 (2) | C18—N4—C19—C20                 | 92.7 (2) |
| C4—N2—C3—C2          | −177.42 (19) | C16—N4—C19—C24              | 106.0 (2) |
| C1—N2—C4—C5          | −93.7 (2) | C18—N4—C19—C24                 | −87.0 (3) |
| C3—N2—C4—C5          | 83.2 (3) | C24—C19—C20—C21                | −0.4 (3) |
| C1—N2—C4—C9          | 86.6 (2) | N4—C19—C20—C21                 | 179.86 (19) |
| C3—N2—C4—C9          | −96.5 (2) | C24—C19—C20—C25                | 179.7 (2) |
| C9—C4—C5—C6          | 1.2 (3)  | N4—C19—C20—C25                 | 0.0 (3) |
| N2—C4—C5—C6          | −178.47 (18) | C19—C20—C21—C22             | 0.6 (4) |
| C9—C4—C5—C10         | −177.9 (2) | C25—C20—C21—C22                | −179.5 (2) |
| N2—C4—C5—C10         | 2.4 (3)  | C20—C21—C22—C23                | −0.5 (4) |
| C4—C5—C6—C7          | −0.8 (3) | C21—C22—C23—C24                | 0.3 (4) |
| C10—C5—C6—C7         | 178.4 (2) | C22—C23—C24—C19                | −0.1 (4) |
| C5—C6—C7—C8          | −0.1 (4) | C22—C23—C24—C28                | −179.8 (2) |
| C6—C7—C8—C9          | 0.6 (4)  | C20—C19—C24—C23                | 0.2 (3) |
| C7—C8—C9—C4          | −0.2 (3) | N4—C19—C24—C23                 | 179.87 (19) |
| C7—C8—C9—C13         | 178.1 (2) | C20—C19—C24—C28                | 179.9 (2) |
| C5—C4—C9—C8          | −0.8 (3) | N4—C19—C24—C28                 | −0.4 (3) |
| N2—C4—C9—C8          | 178.94 (18) | C21—C20—C25—C27             | −63.4 (3) |
| C5—C4—C9—C13         | −179.07 (19) | C19—C20—C25—C27             | 116.5 (2) |

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N2—C4—C9—C13 0.6 (3) C21—C20—C25—C26 60.8 (3)
C6—C5—C10—C11 −73.6 (3) C19—C20—C25—C26 −119.3 (2)
C4—C5—C10—C11 105.5 (3) C23—C24—C28—C29 59.7 (3)
C6—C5—C10—C12 52.9 (3) C19—C24—C28—C29 −120.0 (3)
C4—C5—C10—C12 −128.0 (3) C23—C24—C28—C30 −64.2 (3)
C8—C9—C13—C14 −72.8 (3) C19—C24—C28—C30 116.1 (3)
C4—C9—C13—C14 105.4 (3) C33B—O1—C31—C32 −174.6 (6)
C8—C9—C13—C15 51.0 (3) C33B—O1—C31—C32 165.9 (6)
C4—C9—C13—C15 −130.8 (2) C31—O1—C33A—C34A 88.5 (8)
C17—N3—C16—N4 −0.3 (2) C33B—O1—C33A—C34A 44.2 (12)
Fe1—N3—C16—N4 0.5 (2) C19—C24—C28—C30 116.1 (7)
C18—N4—C16—N3 0.5 (2) C31—O1—C33B—C34B −46.0 (12)

Symmetry code: (i) −x+1, −y+2, −z+1.

**Hydrogen-bond geometry (Å, †)**

Cg2 and Cg3 are the centroids of rings N3/N4/C16–C18 and C4–C9, respectively.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| C1—H1···Br1i | 0.95 | 2.76 | 3.399 (2) | 125 |
| C2—H2···Br1 | 0.95 | 2.89 | 3.479 (2) | 121 |
| C16—H16···Br1 | 0.95 | 2.86 | 3.4119 (18) | 118 |
| C17—H17···Br1i | 0.95 | 3.02 | 3.542 (2) | 116 |
| C18—H18···O1ii | 0.95 | 2.40 | 3.337 (3) | 170 |
| C15—H15A···Cg3iii | 0.98 | 2.92 | 3.801 (3) | 150 |
| C25—H25···Cg2 | 1.00 | 2.61 | 3.413 (2) | 137 |
| C26—H26A···Cg3iv | 0.98 | 2.87 | 3.682 (3) | 140 |
| C34B—H34E···Cg2v | 0.98 | 2.92 | 3.627 (9) | 130 |

Symmetry codes: (i) −x+1, −y+2, −z+1; (ii) −x+2, −y+2, −z+1; (iii) −x+1, −y+3, −z+1; (iv) −x+1, −y+2, −z+2; (v) x, y, z−4.