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1,1′-Bis(4-bromophenyl)-3,3′-diphenylferrocene

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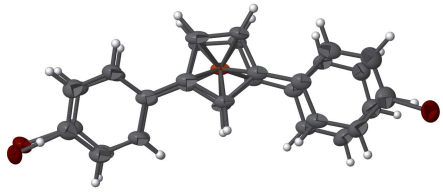
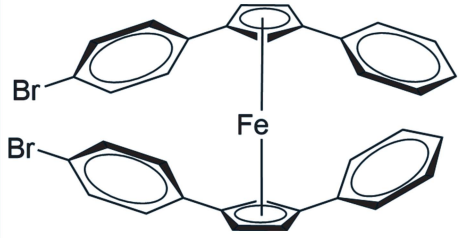
In the title compound, $[Fe(C_{17}H_{12}Br)_2]$, the Fe^{II} atom is sandwiched between the eclipsed five-membered rings, with Fe···ring centroid distances of 1.649 (3) and 1.652 (3) Å. In one of the ligands, the Br atom is disordered over two locations [site occupancies = 0.839 (2) and 0.161 (2)].

3D view



Chemical scheme



Structure description

Substituted ferrocenes have been investigated for their applications in molecular machines (Muraoka *et al.*, 2003), as arylation catalysts (Schmiel & Butenschön, 2017), and to moderate the burning rates of composited solid propellants (Liu *et al.*, 2015). In an effort to provide a structurally simple starting material for further diversification, the title ferrocene complex, with each cyclopentadienyl ligand bearing a phenyl and 4-bromophenyl susbstituent at its 1 and 3 positions, was synthesized.

The title compound (Fig. 1) crystallizes in the orthorhombic space group $Pna2_1$ with one molecule per asymmetric unit. The compound consists of two 1-(4-bromophenyl)-3-phenylcyclopentadienyl ligands with the Fe^{II} atom sandwiched between the cyclopentadienyl ligands. The distances between the cyclopentadienyl centroids and the Fe^{II} atom are 1.649 (3) and 1.652 (3) Å: the five-membered rings are almost eclipsed. The phenyl substituents are twisted slightly with respect to the cyclopentadienyl cores, with deviations of the ring planes ranging from 10.5 (3) to 19.6 (3)°. The main disorder component of Br1 and Br1′ both lie at the same end of the molecule.

Synthesis and crystallization

The title compound was synthesized following a modified literature procedure (Peloquin *et al.*, 2012). A solution of 3-(4-bromophenyl)-cyclopent-2-en-1-one (43.40 g, 183.0 mmol) in THF (500 ml) under N_2 was added dropwise over 15 min to vigorously stirred PhMgCl in THF (2.0 *M*, 119.0 ml, 238.0 mmol) under N_2. The resulting brown reaction mixture

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{17}H_{12}Br)_2]$
M_r	648.20
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	100
a, b, c (Å)	24.2914 (17), 14.3317 (10), 7.5014 (5)
V (Å^3)	2611.5 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.66
Crystal size (mm)	0.19 × 0.14 × 0.08
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2017)
T_{min}, T_{max}	0.50, 0.75
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53974, 6454, 5283
R_{int}	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.103, 1.07
No. of reflections	6454
No. of parameters	344
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.44, −0.77
Absolute structure	Flack x determined using 2036 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.052 (6)

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae, *et al.*, 2008) and *publCIF* (Westrip, 2010).

was allowed to stir at room temperature for 15 h under N_2, exposed to air, and the THF was removed by rotary vacuum to give a brown residue. The brown residue was taken up and vigorously stirred in a mixture of water (300 ml) and Et_2O (500 ml). Addition of 1 *M* H_2SO_4 (61.3 ml, 61.3 mmol) resulted in a brown Et_2O layer and a clear water layer, which was stirred for an additional 5 min. The brown Et_2O layer was separated and washed sequentially with saturated $NaHCO_3$ (3 × 200 ml), water (2 × 200 ml), and saturated brine (200 ml). The organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum to afford a golden-colored oil, which was recrystallized by dissolving in boiling hot absolute ethanol (300 ml) and cooling (268 K). Vacuum filtration, washing with cold absolute ethanol (20 ml), and vacuum drying afforded the target compound as yellow crystalline flakes (45.7 g, 84%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.61–7.35 (*m*, 10H), 6.64 (*d*, 1H, J = 5.5 Hz), 3.56 (*d*, 2H, J = 17 Hz).

Metallation was accomplished *via* a modified literature procedure (Hosono *et al.*, 2013). To a solution of 1-(4-bromophenyl)-3-phenyl-cyclopentadiene (4.80 g, 16.2 mmol) in THF (100 ml) at 273 K, KO*t*-Bu (2.13 g, 19.0 mmol) was added and the mixture was allowed to gradually warm to room temperature and stir for 7 h. The resulting reddish-brown solution was added *via* cannula transfer to a suspension of

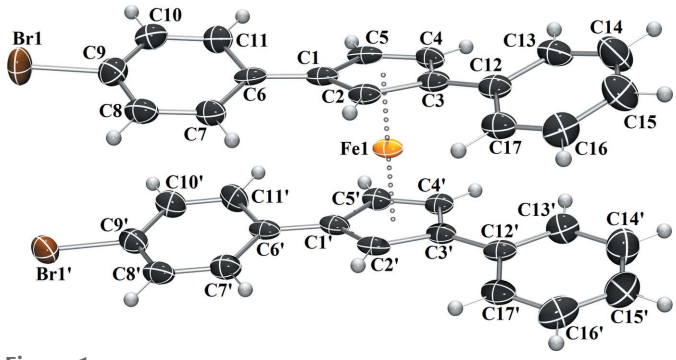


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are shown at the 50% probability level. Only the primary disorder component for Br1 and associated H atoms is shown.

$FeCl_2$ (2.02 g, 15.9 mmol) in THF (50 ml) at 273 K. After stirring at room temperature under N_2 for 18 hrs, 500 ml of water was added to the reaction mixture. The mixture was extracted with CH_2Cl_2 (2 × 250 ml), dried over $MgSO_4$, and evaporated to dryness under reduced pressure. The resulting solid was recrystallized from Et_2O solution to yield the target product as an orange solid (2.104 g, 40%). Crystals suitable for X-ray diffraction were obtained by layering a saturated dichloromethane solution with acetonitrile. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.26–7.16 (*m*, 12H), 7.01 (*d*, 2H, J = 9.0 Hz), 6.95 (*d*, 2H, J = 8.0 Hz), 4.72 (*br s*, 2H), 4.50 (*br d*, 2H, J = 10 Hz), 4.43 (*br s*, 2H).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Atom Br1 is disordered over two positions, bound to C9 and C15, with a refined occupancy of 0.839 (2) at the C9 position.

Funding information

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full crystallographic data

IUCrData (2019). **4**, x190487 [https://doi.org/10.1107/S2414314619004875]

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(I)

Crystal data

$[Fe(C_{17}H_{12}Br)_2]$
M_r = 648.20
Orthorhombic, $Pna2_1$
a = 24.2914 (17) Å
b = 14.3317 (10) Å
c = 7.5014 (5) Å
V = 2611.5 (3) Å^3
Z = 4
$F(000)$ = 1296
D_x = 1.649 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7252 reflections
θ = 2.2–22.9°
μ = 3.66 mm^{-1}
T = 100 K
Plate, translucent orange
0.19 × 0.14 × 0.08 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.50, T_{max} = 0.75
53974 measured reflections
6454 independent reflections
5283 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −32→32
k = −19→19
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.103
S = 1.07
6454 reflections
344 parameters
6 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 3.9647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}
Absolute structure: Flack x determined using 2036 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.052 (6)

Special details

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

Refinement. Bromine atom Br1 was modeled across two positions, bound to C9 and C15, with final refined occupancy of 0.83925 at the C9 position. An attempt to bring the Br1A-C9 bond length (1.561) to a more reasonable length was made using DFIX, but the small occupancy of the C15 site limited the effectiveness of this method. The final Flack parameter 0.052 applies only to the smaller disordered part (the main disordered part is not chiral). The main disordered part is not chiral, and any amount of chiral product would have been formed as a racemic mixture during synthesis.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.66063 (4)	0.92233 (6)	0.17341 (14)	0.0445 (3)	0.839 (2)
Br1A	0.51480 (18)	0.0149 (3)	0.1444 (7)	0.0477 (17)	0.161 (2)
Br1′	0.77282 (3)	0.88889 (5)	0.61250 (11)	0.04133 (18)	
Fe1	0.59400 (3)	0.45241 (6)	0.60272 (13)	0.02673 (19)	
C1	0.5686 (2)	0.5472 (5)	0.4128 (8)	0.0302 (15)	
C2	0.5808 (3)	0.4582 (5)	0.3366 (8)	0.0281 (14)	
H2	0.608217	0.446759	0.248916	0.034*	
C3	0.5452 (3)	0.3885 (5)	0.4131 (8)	0.0307 (15)	
C4	0.5123 (2)	0.4359 (5)	0.5433 (9)	0.0290 (14)	
H4	0.485344	0.407651	0.617479	0.035*	
C5	0.5263 (2)	0.5305 (5)	0.5434 (9)	0.0336 (16)	
H5	0.510318	0.576675	0.618071	0.04*	
C6	0.5919 (2)	0.6370 (5)	0.3646 (8)	0.0280 (14)	
C7	0.6411 (3)	0.6440 (5)	0.2692 (9)	0.0332 (15)	
H7	0.660541	0.588559	0.239819	0.04*	
C8	0.6623 (3)	0.7281 (5)	0.2167 (10)	0.0387 (17)	
H8	0.696148	0.731057	0.153696	0.046*	
C9	0.6336 (3)	0.8084 (5)	0.2568 (10)	0.0405 (17)	
H9	0.647462	0.866911	0.217657	0.049*	0.161 (2)
C10	0.5849 (3)	0.8054 (5)	0.3533 (10)	0.0397 (17)	
H10	0.565861	0.8613	0.382097	0.048*	
C11	0.5646 (3)	0.7206 (5)	0.4065 (9)	0.0351 (16)	
H11	0.531359	0.718346	0.472983	0.042*	
C12	0.5403 (3)	0.2908 (5)	0.3615 (8)	0.0331 (15)	
C13	0.4930 (3)	0.2384 (6)	0.4070 (10)	0.0418 (18)	
H13	0.465195	0.266712	0.47761	0.05*	
C14	0.4862 (3)	0.1486 (6)	0.3527 (12)	0.054 (2)	
H14	0.453349	0.115966	0.381278	0.065*	
C15	0.5274 (3)	0.1046 (6)	0.2552 (12)	0.052 (2)	
H15	0.522978	0.041609	0.218143	0.062*	0.839 (2)
C16	0.5750 (3)	0.1529 (5)	0.2123 (10)	0.0421 (18)	
H16	0.603479	0.122737	0.147555	0.051*	
C17	0.5810 (3)	0.2440 (6)	0.2629 (9)	0.0365 (16)	
H17	0.61364	0.276524	0.23057	0.044*	
C1′	0.6620 (3)	0.5083 (5)	0.7288 (8)	0.0295 (14)	
C2′	0.6750 (2)	0.4217 (5)	0.6481 (8)	0.0287 (14)	
H2′	0.702109	0.412482	0.558641	0.034*	
C3′	0.6406 (2)	0.3497 (5)	0.7226 (8)	0.0278 (14)	
C4′	0.6055 (3)	0.3955 (5)	0.8476 (8)	0.0284 (14)	

H4′	0.577765	0.365716	0.916606	0.034*
C5′	0.6180 (3)	0.4907 (5)	0.8532 (8)	0.0291 (14)
H5′	0.600468	0.535922	0.926426	0.035*
C6′	0.6879 (2)	0.5988 (5)	0.6958 (8)	0.0299 (14)
C7′	0.7369 (2)	0.6062 (5)	0.5964 (11)	0.0348 (14)
H7′	0.752997	0.551791	0.546345	0.042*
C8′	0.7620 (3)	0.6925 (5)	0.5709 (9)	0.0379 (18)
H8′	0.795343	0.697049	0.505082	0.045*
C9′	0.7382 (3)	0.7706 (5)	0.6419 (8)	0.0351 (16)
C10′	0.6895 (3)	0.7662 (5)	0.7365 (9)	0.0371 (16)
H10′	0.673468	0.821246	0.784335	0.044*
C11′	0.6646 (3)	0.6810 (5)	0.7603 (9)	0.0352 (16)
H11′	0.630518	0.678081	0.822461	0.042*
C12′	0.6427 (2)	0.2504 (5)	0.6802 (8)	0.0311 (14)
C13′	0.6021 (3)	0.1888 (5)	0.7454 (10)	0.0403 (17)
H13′	0.572269	0.212889	0.813014	0.048*
C14′	0.6050 (3)	0.0925 (6)	0.7123 (13)	0.052 (2)
H14′	0.577072	0.052326	0.757026	0.062*
C15′	0.6481 (3)	0.0558 (5)	0.6151 (13)	0.0493 (18)
H15′	0.650562	−0.009517	0.595725	0.059*
C16′	0.6878 (4)	0.1156 (6)	0.5457 (10)	0.048 (2)
H16′	0.717118	0.091094	0.476041	0.057*
C17′	0.6849 (3)	0.2106 (5)	0.5778 (9)	0.0360 (17)
H17′	0.712463	0.250117	0.528919	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0512 (5)	0.0259 (4)	0.0565 (6)	−0.0057 (4)	0.0129 (4)	0.0011 (4)
Br1A	0.042 (3)	0.042 (3)	0.058 (4)	−0.0072 (19)	−0.005 (2)	−0.006 (2)
Br1′	0.0317 (3)	0.0501 (4)	0.0422 (4)	−0.0068 (3)	0.0022 (4)	0.0074 (4)
Fe1	0.0192 (4)	0.0440 (5)	0.0170 (3)	0.0062 (3)	0.0000 (4)	0.0042 (5)
C1	0.020 (3)	0.051 (4)	0.020 (3)	0.009 (3)	−0.002 (2)	0.005 (3)
C2	0.021 (3)	0.046 (4)	0.017 (3)	0.008 (3)	0.000 (2)	0.003 (3)
C3	0.023 (3)	0.049 (4)	0.020 (3)	0.006 (3)	−0.002 (2)	0.007 (3)
C4	0.019 (3)	0.045 (4)	0.023 (3)	0.001 (3)	0.002 (2)	0.006 (3)
C5	0.019 (3)	0.061 (5)	0.021 (3)	0.014 (3)	0.000 (2)	0.006 (3)
C6	0.022 (3)	0.045 (4)	0.018 (3)	0.011 (3)	−0.005 (2)	0.002 (3)
C7	0.026 (3)	0.047 (4)	0.027 (3)	0.003 (3)	0.004 (3)	0.005 (3)
C8	0.026 (3)	0.055 (4)	0.035 (4)	0.006 (3)	0.001 (3)	0.006 (3)
C9	0.039 (4)	0.046 (4)	0.036 (4)	0.000 (3)	−0.002 (3)	0.009 (3)
C10	0.035 (4)	0.044 (4)	0.040 (4)	0.009 (3)	−0.003 (3)	0.002 (3)
C11	0.033 (4)	0.044 (4)	0.029 (3)	0.002 (3)	0.003 (3)	0.003 (3)
C12	0.030 (4)	0.047 (4)	0.022 (3)	0.004 (3)	−0.005 (3)	0.005 (3)
C13	0.027 (3)	0.060 (5)	0.038 (4)	0.000 (3)	−0.002 (3)	0.006 (4)
C14	0.038 (4)	0.057 (5)	0.068 (6)	−0.011 (4)	−0.002 (4)	−0.006 (5)
C15	0.048 (5)	0.055 (5)	0.052 (5)	−0.010 (4)	−0.005 (4)	−0.010 (4)
C16	0.048 (4)	0.045 (4)	0.034 (4)	0.006 (4)	0.002 (3)	−0.007 (3)

C17	0.027 (3)	0.054 (5)	0.029 (4)	0.004 (3)	0.003 (3)	0.007 (3)
C1′	0.021 (3)	0.046 (4)	0.022 (3)	0.002 (3)	−0.005 (2)	0.002 (3)
C2′	0.018 (3)	0.050 (4)	0.017 (3)	0.008 (3)	−0.001 (2)	−0.001 (3)
C3′	0.022 (3)	0.044 (4)	0.017 (3)	0.004 (3)	−0.002 (2)	0.004 (3)
C4′	0.025 (3)	0.043 (4)	0.017 (3)	0.004 (3)	−0.002 (2)	0.007 (3)
C5′	0.025 (3)	0.044 (4)	0.018 (3)	0.003 (3)	0.000 (2)	0.001 (3)
C6′	0.021 (3)	0.051 (4)	0.018 (3)	0.005 (3)	−0.003 (2)	0.004 (3)
C7′	0.028 (3)	0.045 (4)	0.031 (3)	0.006 (3)	0.002 (3)	0.002 (4)
C8′	0.023 (3)	0.058 (5)	0.032 (5)	0.004 (3)	0.001 (3)	0.011 (3)
C9′	0.029 (3)	0.050 (4)	0.026 (4)	−0.003 (3)	−0.002 (3)	0.004 (3)
C10′	0.031 (4)	0.047 (4)	0.034 (4)	0.003 (3)	0.006 (3)	−0.005 (3)
C11′	0.027 (3)	0.046 (4)	0.033 (4)	−0.002 (3)	0.011 (3)	−0.001 (3)
C12′	0.026 (3)	0.048 (4)	0.020 (3)	0.008 (3)	−0.004 (3)	0.005 (3)
C13′	0.040 (4)	0.047 (4)	0.034 (4)	0.005 (3)	0.007 (3)	−0.001 (3)
C14′	0.051 (5)	0.044 (5)	0.061 (6)	0.002 (4)	0.012 (4)	0.000 (4)
C15′	0.058 (4)	0.046 (4)	0.044 (4)	0.006 (4)	0.001 (5)	0.003 (4)
C16′	0.055 (5)	0.051 (5)	0.037 (4)	0.018 (4)	−0.001 (4)	−0.007 (4)
C17′	0.028 (3)	0.054 (4)	0.025 (4)	0.004 (3)	−0.001 (3)	0.007 (3)

Geometric parameters (Å, º)

Br1—C9	1.868 (8)	C14—C15	1.391 (12)
Br1A—C15	1.561 (9)	C14—H14	0.95
Br1′—C9′	1.906 (7)	C15—C16	1.385 (11)
Fe1—C2	2.023 (6)	C15—H15	0.95
Fe1—C4′	2.029 (6)	C16—C17	1.367 (11)
Fe1—C5	2.039 (6)	C16—H16	0.95
Fe1—C5′	2.042 (6)	C17—H17	0.95
Fe1—C2′	2.044 (5)	C1′—C2′	1.417 (9)
Fe1—C4	2.048 (6)	C1′—C5′	1.441 (9)
Fe1—C3′	2.063 (6)	C1′—C6′	1.463 (9)
Fe1—C1	2.063 (6)	C2′—C3′	1.439 (9)
Fe1—C1′	2.064 (6)	C2′—H2′	0.95
Fe1—C3	2.066 (7)	C3′—C4′	1.427 (9)
C1—C2	1.429 (10)	C3′—C12′	1.459 (9)
C1—C5	1.440 (9)	C4′—C5′	1.398 (9)
C1—C6	1.452 (10)	C4′—H4′	0.95
C2—C3	1.441 (9)	C5′—H5′	0.95
C2—H2	0.95	C6′—C11′	1.394 (9)
C3—C4	1.434 (9)	C6′—C7′	1.409 (9)
C3—C12	1.457 (10)	C7′—C8′	1.391 (10)
C4—C5	1.397 (10)	C7′—H7′	0.95
C4—H4	0.95	C8′—C9′	1.369 (10)
C5—H5	0.95	C8′—H8′	0.95
C6—C7	1.396 (9)	C9′—C10′	1.380 (9)
C6—C11	1.405 (9)	C10′—C11′	1.375 (10)
C7—C8	1.367 (10)	C10′—H10′	0.95
C7—H7	0.95	C11′—H11′	0.95

C8—C9	1.379 (10)	C12′—C17′	1.404 (9)
C8—H8	0.95	C12′—C13′	1.411 (10)
C9—C10	1.388 (10)	C13′—C14′	1.404 (11)
C9—H9	0.95	C13′—H13′	0.95
C10—C11	1.370 (10)	C14′—C15′	1.379 (11)
C10—H10	0.95	C14′—H14′	0.95
C11—H11	0.95	C15′—C16′	1.393 (12)
C12—C17	1.406 (9)	C15′—H15′	0.95
C12—C13	1.414 (10)	C16′—C17′	1.384 (11)
C13—C14	1.360 (12)	C16′—H16′	0.95
C13—H13	0.95	C17′—H17′	0.95

C2—Fe1—C4′	158.6 (3)	C9—C10—H10	120.5
C2—Fe1—C5	68.5 (3)	C10—C11—C6	121.4 (6)
C4′—Fe1—C5	121.9 (3)	C10—C11—H11	119.3
C2—Fe1—C5′	160.4 (3)	C6—C11—H11	119.3
C4′—Fe1—C5′	40.2 (3)	C17—C12—C13	116.4 (7)
C5—Fe1—C5′	106.5 (3)	C17—C12—C3	122.7 (6)
C2—Fe1—C2′	109.0 (2)	C13—C12—C3	120.9 (6)
C4′—Fe1—C2′	68.3 (2)	C14—C13—C12	122.0 (7)
C5—Fe1—C2′	158.6 (3)	C14—C13—H13	119.0
C5′—Fe1—C2′	68.3 (2)	C12—C13—H13	119.0
C2—Fe1—C4	68.7 (3)	C13—C14—C15	120.0 (8)
C4′—Fe1—C4	106.5 (3)	C13—C14—H14	120.0
C5—Fe1—C4	40.0 (3)	C15—C14—H14	120.0
C5′—Fe1—C4	120.5 (3)	C16—C15—C14	119.7 (8)
C2′—Fe1—C4	160.7 (3)	C16—C15—Br1A	116.9 (7)
C2—Fe1—C3′	123.1 (3)	C14—C15—Br1A	120.8 (7)
C4′—Fe1—C3′	40.8 (2)	C16—C15—H15	120.2
C5—Fe1—C3′	158.4 (3)	C14—C15—H15	120.2
C5′—Fe1—C3′	68.5 (3)	C17—C16—C15	120.2 (7)
C2′—Fe1—C3′	41.0 (3)	C17—C16—H16	119.9
C4—Fe1—C3′	123.0 (3)	C15—C16—H16	119.9
C2—Fe1—C1	40.9 (3)	C16—C17—C12	121.7 (7)
C4′—Fe1—C1	158.6 (3)	C16—C17—H17	119.2
C5—Fe1—C1	41.1 (2)	C12—C17—H17	119.2
C5′—Fe1—C1	122.9 (3)	C2′—C1′—C5′	106.8 (6)
C2′—Fe1—C1	123.0 (3)	C2′—C1′—C6′	127.5 (6)
C4—Fe1—C1	68.6 (3)	C5′—C1′—C6′	125.8 (6)
C3′—Fe1—C1	159.2 (2)	C2′—C1′—Fe1	69.0 (3)
C2—Fe1—C1′	124.2 (3)	C5′—C1′—Fe1	68.6 (4)
C4′—Fe1—C1′	68.4 (3)	C6′—C1′—Fe1	127.6 (4)
C5—Fe1—C1′	122.2 (3)	C1′—C2′—C3′	109.4 (5)
C5′—Fe1—C1′	41.1 (2)	C1′—C2′—Fe1	70.6 (3)
C2′—Fe1—C1′	40.4 (3)	C3′—C2′—Fe1	70.2 (3)
C4—Fe1—C1′	156.9 (3)	C1′—C2′—H2′	125.3
C3′—Fe1—C1′	68.8 (3)	C3′—C2′—H2′	125.3
C1—Fe1—C1′	107.5 (3)	Fe1—C2′—H2′	125.5

C2—Fe1—C3	41.2 (3)	C4′—C3′—C2′	105.8 (6)
C4′—Fe1—C3	121.6 (3)	C4′—C3′—C12′	127.7 (6)
C5—Fe1—C3	68.3 (3)	C2′—C3′—C12′	126.4 (6)
C5′—Fe1—C3	156.4 (3)	C4′—C3′—Fe1	68.3 (3)
C2′—Fe1—C3	124.8 (3)	C2′—C3′—Fe1	68.8 (3)
C4—Fe1—C3	40.8 (3)	C12′—C3′—Fe1	128.2 (4)
C3′—Fe1—C3	107.4 (3)	C5′—C4′—C3′	109.8 (6)
C1—Fe1—C3	69.2 (3)	C5′—C4′—Fe1	70.4 (4)
C1′—Fe1—C3	161.2 (3)	C3′—C4′—Fe1	70.9 (3)
C2—C1—C5	105.8 (6)	C5′—C4′—H4′	125.1
C2—C1—C6	127.6 (6)	C3′—C4′—H4′	125.1
C5—C1—C6	126.6 (6)	Fe1—C4′—H4′	125.2
C2—C1—Fe1	68.0 (4)	C4′—C5′—C1′	108.2 (6)
C5—C1—Fe1	68.5 (4)	C4′—C5′—Fe1	69.4 (4)
C6—C1—Fe1	129.7 (4)	C1′—C5′—Fe1	70.3 (4)
C1—C2—C3	109.6 (6)	C4′—C5′—H5′	125.9
C1—C2—Fe1	71.0 (4)	C1′—C5′—H5′	125.9
C3—C2—Fe1	70.9 (3)	Fe1—C5′—H5′	126.0
C1—C2—H2	125.2	C11′—C6′—C7′	117.6 (6)
C3—C2—H2	125.2	C11′—C6′—C1′	121.0 (6)
Fe1—C2—H2	124.4	C7′—C6′—C1′	121.4 (6)
C4—C3—C2	106.1 (6)	C8′—C7′—C6′	120.7 (6)
C4—C3—C12	126.2 (6)	C8′—C7′—H7′	119.7
C2—C3—C12	127.6 (6)	C6′—C7′—H7′	119.7
C4—C3—Fe1	68.9 (4)	C9′—C8′—C7′	119.1 (6)
C2—C3—Fe1	67.8 (4)	C9′—C8′—H8′	120.4
C12—C3—Fe1	131.0 (5)	C7′—C8′—H8′	120.4
C5—C4—C3	108.9 (6)	C8′—C9′—C10′	121.7 (6)
C5—C4—Fe1	69.7 (4)	C8′—C9′—Br1′	119.7 (5)
C3—C4—Fe1	70.3 (4)	C10′—C9′—Br1′	118.6 (5)
C5—C4—H4	125.5	C11′—C10′—C9′	119.0 (7)
C3—C4—H4	125.5	C11′—C10′—H10′	120.5
Fe1—C4—H4	126.1	C9′—C10′—H10′	120.5
C4—C5—C1	109.6 (6)	C10′—C11′—C6′	121.7 (6)
C4—C5—Fe1	70.4 (4)	C10′—C11′—H11′	119.1
C1—C5—Fe1	70.4 (3)	C6′—C11′—H11′	119.1
C4—C5—H5	125.2	C17′—C12′—C13′	116.5 (7)
C1—C5—H5	125.2	C17′—C12′—C3′	122.7 (6)
Fe1—C5—H5	125.7	C13′—C12′—C3′	120.8 (6)
C7—C6—C11	117.2 (6)	C14′—C13′—C12′	121.3 (7)
C7—C6—C1	121.7 (6)	C14′—C13′—H13′	119.3
C11—C6—C1	121.0 (6)	C12′—C13′—H13′	119.3
C8—C7—C6	122.1 (7)	C15′—C14′—C13′	120.3 (8)
C8—C7—H7	118.9	C15′—C14′—H14′	119.8
C6—C7—H7	118.9	C13′—C14′—H14′	119.8
C7—C8—C9	118.9 (7)	C14′—C15′—C16′	119.4 (8)
C7—C8—H8	120.6	C14′—C15′—H15′	120.3
C9—C8—H8	120.6	C16′—C15′—H15′	120.3

C8—C9—C10	121.2 (7)	C17′—C16′—C15′	120.3 (7)
C8—C9—Br1	118.7 (6)	C17′—C16′—H16′	119.8
C10—C9—Br1	120.1 (6)	C15′—C16′—H16′	119.8
C8—C9—H9	119.4	C16′—C17′—C12′	122.2 (7)
C10—C9—H9	119.4	C16′—C17′—H17′	118.9
C11—C10—C9	119.1 (7)	C12′—C17′—H17′	118.9
C11—C10—H10	120.5		