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Crystal structure analysis of two Ferrocene derivatives

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Abstract: Two Ferrocene compounds (FERR1 and FERR2) were crystallized by slow evaporation method. Crystal data were collected using BRUKER SMART APEX II CCD X-ray diffractometer. The structures were solved by direct methods and refined on F^2 by full-matrix least-squares procedures using the SHELXL programs. FERR1 (1-N-methyl-spiro-[2',11']-indeno-[1,26]-quinoxaline-3-ferrocenyl-4-thiophene pyrrolidine) crystallizes in triclinic $P\bar{1}$ space group and the final R is 0.052. FERR2 (1-N-methyl-spiro-[2',11']-indeno-[1,26]-quinoxaline-3-ferrocenoyl-4-ferrocene pyrrolidine) crystallizes in monoclinic $P2_1$ space group and the final R value is 0.063.
Key Words: Ferrocene, crystal structure.

Introduction

Ferrocene derivatives are organometallic compounds consisting two cyclopentadienyl rings bound at opposite sides of a central metal atom. The stability of Ferrocene in aqueous and aerobic media, the accessibility of a large variety of derivatives, and its favourable electrochemical properties have made ferrocenyl compounds very popular molecules for biological applications[1-8]. The use of Ferrocene in medicinal applications is an active research area. Many reports have shown that some Ferrocene derivatives are highly active *in vitro* and *in vivo*, against several diseases including fungal and bacterial infections[9,11], malaria[10,12,13], human immunodeficiency virus (HIV)[14] and some ferrocenium salts exhibit anticancer activity, and an experimental drug has been reported which is a ferrocenyl version of tamoxifen[15]. The idea is that the tamoxifen will bind to the estrogen binding sites, resulting in a cytotoxicity effect[16].

Experimental

X-ray Structure Determination

Single crystal of the compound suitable for x-ray diffraction was obtained by slow evaporation method. Three dimensional intensity data were collected on a Bruker[17] SMART APEX CCD Diffractometer using graphite monochromatized Mo-Kα radiation (λ= 0.71073 Å) at the CAS in Crystallography and Biophysics, University of Madras, Chennai. The structures were solved by direct methods and refined on F^2 by full-matrix least-squares procedures using the *SHELXL* programs[18]. All the non-hydrogen atoms were refined using anisotropic thermal parameters. The hydrogen atoms were included in the structure factor calculation at idealized positions by using a riding model, but not refined. Images were created with the ORTEP-3[19]. The crystallographic data for the compounds are listed in Table 1.

Table 1 Crystal Data of FERR1 and FERR2

Particulars	**FERR1**	**FERR2**
Empirical formula	C_{34} H_{27} Fe N_3 O S	C_{40} H_{33} Fe_2 N_3 O
Formula weight	581.50	683.39
Temperature (K)	293(2)	293(2)
Wavelength	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	P $\bar{1}$	P 2_1
Unit cell dimensions	a = 10.20(5) Å α= 77.439(5)° b = 12.06(5) Å β= 89.709(5)° c = 12.52(5) Å γ = 68.180(5)°	a = 10.89(3) α= 90° b = 1118(5) β= 102.187(2)° c = 13.21(4) γ = 90°
Volume ($Å^3$)	1390.5(11)	1572.62(10)
Z	2	2
Density (g/cm^{-1})	1.389	1.443
Absorption coefficient (mm^{-1})	0.650	0.960
F(000)	604	708
Crystal size (mm^3)	0.2×0.2×0.2	0.2×0.2×0.2
Theta range for data collection	1.67 to 28.59°	1.58 to 28.41°.
Index ranges	-13<=h<=13, -15<=k<=16, -16<=l<=16	-14<=h<=14, -14<=k<=14, -16<=l<=17
Reflections collected	25914	14701
Independent reflections	7025 [R(int) = 0.0282]	6794 [R(int) = 0.0253]
Completeness to theta = 28.33°	98.9 %	97.5 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7025 / 0 / 362	6794 / 1 / 417
Goodness-of-fit on F^2	1.053	1.097
Final R indices [I>2sigma(I)]	R1 = 0.052, wR2 = 0.1714	R1 = 0.063, wR2 = 0.1537
R indices (all data)	R1 = 0.0595, wR2 = 0.1802	R1 = 0.0825, wR2 = 0.1700
Extinction coefficient	0	0.0000(11)
Largest diff. peak and hole ($eÅ^{-3}$)	1.456 and -0.909	1.881 and -0.336

Synthesis of the compound

Synthesis of FERR1

A mixture of ferrocenoyl-2-thiophene derived dipolerophile (1 mmol) was reacted with ninhydrin (1 mmol), 2-phenylenediamine (1 mmol) and sarcosine (1 mmol) in 10ml of methanol at 60-65 ° C, and refluxed for 4 hours. The reaction was monitored by TLC until the starting material diminished. The pure compound was obtained by column chromatography using 8:2 ratio of hexane and ethyl acetate. The solvent content was removed by rotary evaporator and the finally yielded 89% of FERR1. It was recrystallized in 9:1 hexane-ethyl acetate mixture by slow evaporation of solvent.

Synthesis of FERR2

A mixture of ferrocenoyl-2-ferrocene derived dipolerophile (1 mmol) was reacted with ninhydrin (1 mmol), 2-phenylenediamine (1 mmol), and sarcosine (1 mmol) in 10 mL of methanol at 60-65 ° C and refluxed for 4 hours. The reaction was monitored by TLC until the starting material diminished. The pure compound was obtained by coloumn chromatography using 8:2 ratio of hexane and ethyl acetate. The solvent content was removed by rotary evaporator and the finally yielded 89% of FERR2. It was recrystallized in 9:1 hexane-ethyl acetate mixture by slow evaporation of solvent.

Results and Discussion

FERR1

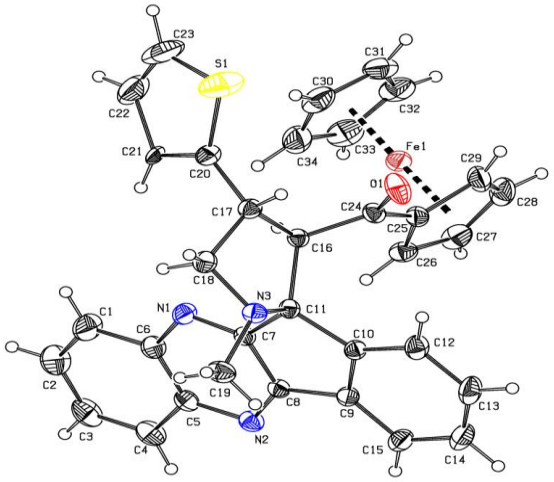

Figure 1. The molecular structure of FERR1 with the atom numbering scheme. Displacement ellipsoids are

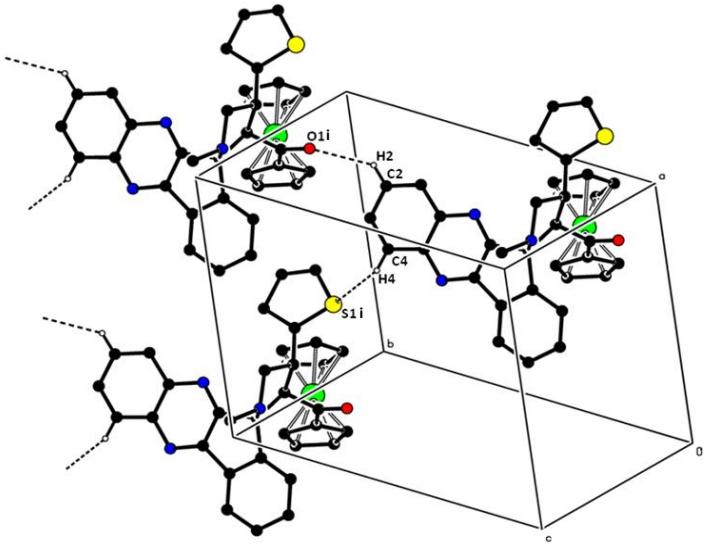

Figure 2. The packing of FERR1 showing the intermolecular C2—H2…O1 and C4—H4…S1 interactions viewed down 'c'-axis and the chain running along 'b'-axis.

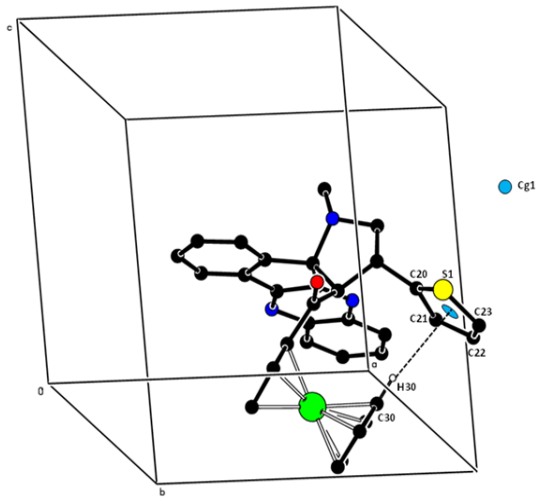

Figure 3. The packing of FERR1 showing the intramolecular C30—H30···Cg1

The ORTEP diagram of FERR1 is shown in Fig. 1. The pyrrolidine ring (N3/C11/C16-C18) adopts a twisted conformation on C18—N3 bond with the puckering parameters q_2 = 0. 413(2) Å, φ = 162.3(4)° and the smallest displacement asymmetric parameter ΔC_2 =1.6 (2)° The indeno-quinoxaline ring system (C1-C6/N1/N2/C7-C15) is essentially planar with a mean deviation of 0.011(2)° at N1 from the least-squares plane defined by the seventeen constituent atoms. The dihedral angle between the indeno-quinoxaline ring system and the pyrrolidine ring is 86.74 (9)°. The thiophene ring (S1/C20-C23) is planar with a mean plane deviation of –0.018°. The Fe1···Cg3 and Fe1···Cg4 distances are 1.6441 (3) and 1.6555 (3) Å, respectively and the Cg3···Fe1···Cg4 angle is 177.47 (7)°, where Cg3 and Cg4 are the centroids of the cyclopentadiene rings C25-C29 and C30-C34, respectively. In the crystal, the molecules are packed by intermolecular C—H···O [C2—H2···O1] and C—H···S [C4—H4···S1] interactions **(**Fig. 2**)** in addition to intramolecular C—H···π interactions [C30—H30···Cg1, where Cg1 is the centroid of the ring atoms S1/C20-23] **(**Fig. 3**)**. In addition, weak C—H···N [C16—H16···N1] and C—H···O [C17—H17···O] interactions are also observed along with van der Waals forces. The hydrogen bonding and non-bonded interactions of FERR1 are presented in Table 2. The selected bond lengths and bond angles are given in tables 3 and 4, respectively.

Table 2 Hydrogen bondings and non-bonded interactions for FERR1

D*—H···*A	***D*—H (Å)**	**H···*A* (Å)**	***D*···*A* (Å)**	***D*—H···*A* (°)**
C2—H2···O1[i]	0.93	2.47	3.208 (4)	136
C4—H4···S1[ii]	0.93	2.84	3.616 (3)	142
C16—H16···N1	0.98	2.61	3.017 (3)	105
C17—H17···O1	0.98	2.32	2.791 (3)	109
C30—H30···Cg1	0.96	2.80	3.647 (3)	152

*Cg1is the centroid of the ring atoms S1-C20-C23.
Symmetry Code: (i) x, 1+y, z, (ii) –1+x, 1+y, z

Table 3 Bond lengths (Å) involving non-hydrogen atoms of FERR1

Atoms	**Bond length (Å)**	**Atoms**	**Bond length (Å)**
C1-C2	137.6(4)	C20-C21	154.7(3)
C1-C6	140.7(3)	C20-S1	168.7(3)
C2-C3	138.5(5)	C21-C22	148.4(4)
C3-C4	136.6(4)	C22-C23	130.1(6)
C4-C5	141.4(3)	C23-S1	166.5(5)
C5-N2	136.8(3)	C24-O1	121.7(3)
C5-C6	141.7(3)	C24-C25	146.6(3)
C6-N1	137.9(3)	C25-C26	142.9(3)
C7-N1	130.2(3)	C25-C29	144.0(3)
C7-C8	142.3(3)	C25-Fe1	203.8(2)
C7-C11	153.0(2)	C26-C27	142.1(3)
C8-N2	131.0(3)	C26-Fe1	203.0(2)
C8-C9	146.4(3)	C27-C28	142.1(5)
C9-C15	138.9(3)	C27-C28	142.1(5)
C9-C10	139.9(3)	C27-Fe1	204.8(3)
C10-C12	139.1(3)	C28-C29	141.0(4)
C10-C11	152.2(3)	C28-Fe1	204.7(3)
C11-N3	147.9(3)	C29-Fe1	204.9(3)
C11-C16	156.9(3)	C30-C34	140.4(5)
C12-C13	138.6(3)	C30-C31	141.1(5)
C13-C14	139.6(4)	C30-Fe1	204.9(3)
C14-C15	138.6(4)	C31-C32	141.5(5)
C16-C24	151.9(3)	C31-Fe1	204.6(3)
C16-C17	155.0(3)	C32-C33	141.0(5)
C17-C20	149.8(3)	C32-Fe1	203.6(3)
C17-C18	152.9(3)	C33-C34	140.3(5)
C18-N3	145.3(3)	C33-Fe1	204.3(3)
C19-N3	146.1(3)	C34-Fe1	204.4(3)

Table 4 Bond angles (°) involving non-hydrogen atoms of FERR1

Atoms	Angle (°)	Atoms	Angle (°)	Atoms	Angle (°)	Atoms	Angle (°)	Atoms	Angle (°)
C2-C1-C6	119.53	C13-C12-C10	118.82	C26-C25-Fe1	69.1512	C33-C34-Fe1	69.8819	C28-Fe1-C27	40.6113
C1-C2-C3	120.93	C12-C13-C14	121.12	C29-C25-Fe1	69.8014	C30-C34-Fe1	70.1218	C26-Fe1-C30	128.5612
C4-C3-C2	120.82	C15-C14-C13	120.62	C24-C25-Fe1	122.1115	C7-N1-C6	114.4818	C32-Fe1-C30	67.8412
C3-C4-C5	120.42	C14-C15-C9	118.12	C27-C26-C25	107.92	C8-N2-C5	114.5018	C25-Fe1-C30	110.3811
N2-C5-C4	119.42	C24-C16-C17	111.7716	C27-C26-Fe1	70.2714	C18-N3-C19	113.0518	C28-Fe1-C27	40.6113
N2-C5-C6	122.2018	C34-C30-C31	108.13	C25-C26-Fe1	69.7112	C18-N3-C11	106.3315	C26-Fe1-C30	128.5612
C4-C5-C6	118.42	C34-C30-Fe1	69.7617	C28-C27-C26	108.12	C19-N3-C11	115.5217	C32-Fe1-C30	67.8412
N1-C6-C1	118.52	C31-C30-Fe1	69.7317	C28-C27-Fe1	69.6516	C23-S1-C20	93.1319	C25-Fe1-C30	110.3811
N1-C6-C5	121.5419	C30-C31-C32	107.53	C26-C27-Fe1	68.9514	C26-Fe1-C32	152.2312	C33-Fe1-C30	67.6114
C1-C6-C5	119.92	C30-C31-Fe1	69.9717	C29-C28-C27	108.72	C26-Fe1-C25	41.149	C34-Fe1-C30	40.1215
N1-C7-C8	123.8218	C24-C16-C11	116.5415	C29-C28-Fe1	69.9615	C32-Fe1-C25	164.2613	C31-Fe1-C30	40.3014
N1-C7-C11	125.2417	C17-C16-C11	104.7216	C27-C28-Fe1	69.7416	C26-Fe1-C33	118.9313	C28-Fe1-C30	154.2815
C8-C7-C11	110.9216	C20-C17-C18	115.1818	C28-C29-C25	107.72	C32-Fe1-C33	40.4415	C27-Fe1-C30	164.8315
N2-C8-C7	123.3718	C20-C17-C16	112.4018	C28-C29-Fe1	69.7616	C25-Fe1-C33	154.7413	C26-Fe1-C29	69.1411
N2-C8-C9	128.6118	C18-C17-C16	104.1716	C25-C29-Fe1	68.9513	C26-Fe1-C34	108.9712	C32-Fe1-C29	125.2114
C7-C8-C9	107.9816	N3-C18-C17	102.3216	C33-Fe1-C28	124.7113	C32-Fe1-C34	67.7514	C25-Fe1-C29	41.259
C15-C9-C10	121.7219	C17-C20-C21	126.6319	C34-Fe1-C28	162.6615	C25-Fe1-C34	121.7511	C33-Fe1-C29	161.9513
C15-C9-C8	129.7919	C17-C20-S1	120.2718	C31-Fe1-C28	118.6814	C33-Fe1-C34	40.1514	C34-Fe1-C29	156.4613
C10-C9-C8	108.4817	C21-C20-S1	112.9616	C26-Fe1-C27	40.7810	C26-Fe1-C31	166.0413	C31-Fe1-C29	108.1214
C12-C10-C9	119.6519	C22-C21-C20	101.32	C32-Fe1-C27	117.3812	C32-Fe1-C31	40.5814	C28-Fe1-C29	40.2712
C12-C10-C11	128.3519	C23-C22-C21	118.43	C32-C31-Fe1	69.3317	C25-Fe1-C31	127.9513	C27-Fe1-C29	68.3212
C9-C10-C11	111.9516	C22-C23-S1	114.23	C33-C32-C31	108.03	C33-Fe1-C31	67.9915	C30-Fe1-C29	121.6614
N3-C11-C10	110.5815	O1-C24-C25	120.6319	C33-C32-Fe1	70.0616	C34-Fe1-C31	67.7215	C32-Fe1-C28	105.8513
N3-C11-C7	113.8216	O1-C24-C16	121.3419	C31-C32-Fe1	70.0917	C26-Fe1-C28	68.7011	C25-Fe1-C28	68.5910
C10-C11-C7	100.4915	C25-C24-C16	117.9717	C34-C33-C32	107.93	C25-Fe1-C27	68.6610	-	-
N3-C11-C16	103.0515	C26-C25-C29	107.62	C34-C33-Fe1	69.9618	C33-Fe1-C27	106.4113	-	-
C10-C11-C16	119.5016	C26-C25-C24	128.02	C32-C33-Fe1	69.5018	C34-Fe1-C27	126.5215	-	-
C7-C11-C16	109.8915	C29-C25-C24	124.22	C33-C34-C30	108.43	C31-Fe1-C27	152.2013	-	-

FERR2

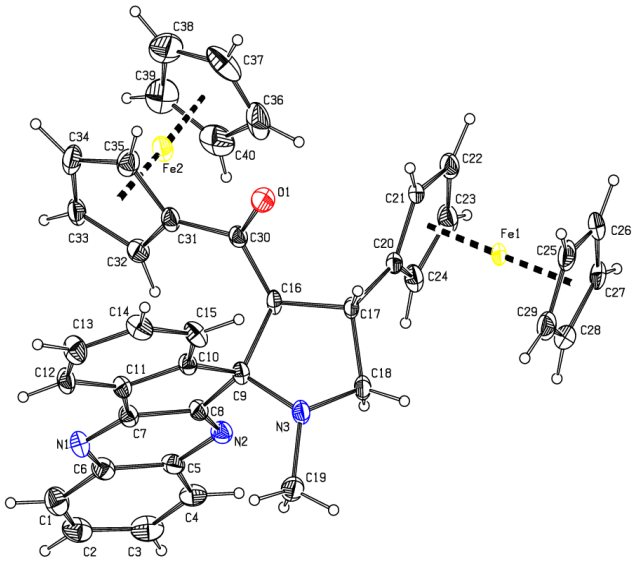

Figure 4. The molecular structure of FERR2 with the atom numbering scheme. Displacement ellipsoids are

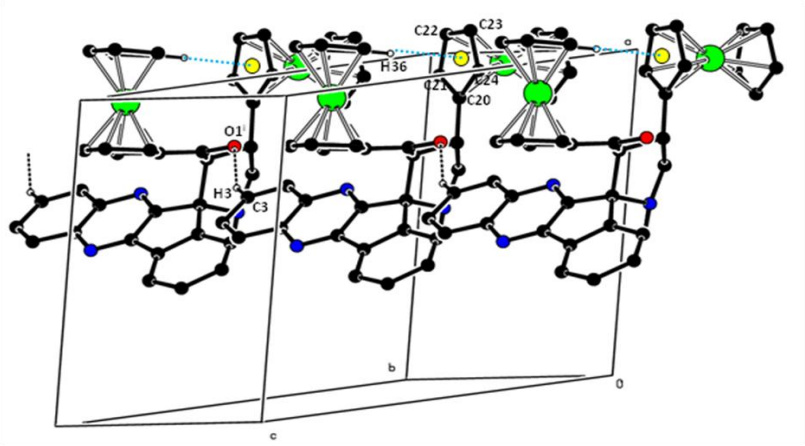

Figure 5. The packing of FERR2 showing the intermolecular C3—H3···O1and intramolecular

The ORTEP diagram of FERR2 is shown in Fig. 4. In FERR2, the pyrrolidine ring (N3/C9/C16-C18) adopts an envelope conformation on atom C18 with the puckering parameters q_2 = 0. 439 (3) Å, φ = 318. 26 (7)° and the smallest displacement asymmetric parameter ΔC_2 = 3.16 (1)°. The indeno-quinoxaline ring (C1-C6/N1/N2/C7-C15) in FERR2 is also essentially planar with a mean deviation of 0.0100 (2)° at C2 from the least-squares plane defined by the seventeen constituent atoms. The dihedral angle between the indeno-quinoxaline ring and the pyrrolidine ring (N3/C9/C16-C18) is 84. 29 (1)°. The Fe1···Cg3 and Fe1···Cg4 distances are 1.6481 and 1.6526 Å whereas Fe2···Cg5 and Fe2···Cg6 distances are 1.6422 and 1.6417 Å, respectively. The Cg3···Fe1···Cg4 and Cg5···Fe2···Cg6 angles are 178.58 and 177.34°, respectively. The molecules are packed within the crystal by intermolecular C—H···O (C3—H3···O1) and C36—H36···Cg1 (where Cg1 is the centroid of the ring atoms C20-24) interactions (Fig. 5) along with other weak non-bonded interactions. The hydrogen bonding and non-bonded interactions of FERR2 are presented in Table 5. The selected bond lengths and bond angles are given in tables 6 and 7, respectively.

Table 5 Hydrogen bondings and non-bonded interactions for FERR2

D*—H⋯*A	***D*—H (Å)**	**H⋯*A* (Å)**	***D*⋯*A* (Å)**	***D*—H⋯*A* (°)**
C3—H3⋯O1[i]	0.93	2.56	3.436 (8)	157
C36—H36⋯Cg1	0.96	2.95	3.871 (9)	171

*Cg1 is the centroids of the ring atoms C20-C24, respectively
Symmetry Code: (i) x, 1+y, z

Table 6 Bond lengths (Å) involving non-hydrogen atoms of FERR1

Atoms	**Bond length (Å)**	**Atoms**	**Bond length (Å)**	**Atoms**	**Bond length (Å)**
C1-C2	132.9(10)	C17-C20	150.5(5)	C30-O1	121.2(6)
C1-C6	140.4(9)	C17-C18	152.5(7)	C30-C31	147.9(6)
C2-C3	141.3(11)	C18-N3	146.9(6)	C31-C35	142.3(8)
C3-C4	135.0(9)	C19-N3	146.0(7)	C31-C32	143.1(8)
C4-C5	140.3(8)	C20-C24	140.8(8)	C31-Fe2	200.3(4)
C5-N2	137.9(7)	C20-C21	141.9(7)	C32-C33	142.8(8)
C5-C6	142.0(8)	C20-Fe1	205.4(4)	C32-Fe2	201.1(5)
C6-N1	137.6(7)	C21-C22	143.2(9)	C33-C34	138.3(10)
C7-N1	132.7(7)	C21-Fe1	204.7(5)	C33-Fe2	204.9(5)
C7-C11	143.7(7)	C22-C23	139.2(12)	C34-C35	139.5(9)
C7-C8	143.5(7)	C22-Fe1	203.5(5)	C34-Fe2	206.4(6)
C8-N2	129.4(7)	C23-C24	140.4(8)	C35-Fe2	205.2(6)
C8-C9	152.5(7)	C23-Fe1	202.1(6)	C36-C37	139.9(14)
C9-N3	147.2(6)	C24-Fe1	203.7(6)	C36-C40	143.0(13)
C9-C10	149.8(6)	C25-C26	138.0(10)	C36-Fe2	202.0(6)
C9-C16	158.6(6)	C25-C29	143.2(10)	C37-C38	138.4(13)
C10-C15	140.8(8)	C25-Fe1	204.8(6)	C37-Fe2	200.1(8)
C10-C11	140.1(6)	C26-C27	139.6(10)	C38-C39	135.4(14)
C11-C12	137.4(7)	C26-Fe1	202.5(6)	C38-Fe2	204.7(8)
C12-C13	138.2(9)	C27-C28	142.2(9)	C39-C40	136.3(13)
C13-C14	138.7(9)	C27-Fe1	205.8(6)	C39-Fe2	202.2(6)
C14-C15	137.0(8)	C28-C29	138.7(11)	C40-Fe2	201.8(7)
C16-C30	149.9(7)	C28-Fe1	203.0(6)	-	-
C16-C17	154.5(5)	C29-Fe1	203.3(5)	-	-

Table 7 Bond angles (°) involving non-hydrogen atoms of FERR2

FERR2											
Atoms	**Angle (°)**	**Atoms**	**Angle (°)**	**Atoms**	**Angle (°)**	**Atoms**	**Angle (°)**	**Atoms**	**Angle (°)**	**Atoms**	**Angle (°)**
C2-C1-C6	122.0(6)	C17-C16-C9	104.9(3)	C27-C28-Fe1	70.7(3)	C38-C39-C40	109.9(10)	C28-Fe1-C25	68.1(3)	C32-Fe2-C39	128.3(4)
C1-C2-C3	120.6(6)	C20-C17-C18	117.6(4)	C28-C29-C25	108.2(5)	C38-C39-Fe2	71.5(5)	C29-Fe1-C25	41.1(3)	C36-Fe2-C39	68.0(4)
C4-C3-C2	119.5(6)	C20-C17-C16	111.0(3)	C28-C29-Fe1	69.9(3)	C40-C39-Fe2	70.1(4)	C24-Fe1-C25	159.1(2)	C40-Fe2-C39	39.4(4)
C3-C4-C5	121.1(6)	C18-C17-C16	101.8(3)	C25-C29-Fe1	70.0(3)	C39-C40-C36	108.1(9)	C22-Fe1-C25	124.0(4)	C31-Fe2-C38	152.8(5)
N2-C5-C4	119.7(5)	N3-C18-C17	100.7(4)	O1-C30-C31	120.9(5)	C39-C40-Fe2	70.5(5)	C21-Fe1-C25	108.8(3)	C37-Fe2-C38	40.0(4)
N2-C5-C6	121.2(5)	C24-C20-C21	107.5(4)	O1-C30-C16	120.9(4)	C36-C40-Fe2	69.3(4)	C23-Fe1-C20	68.1(2)	C32-Fe2-C38	163.6(4)
C4-C5-C6	119.1(5)	C24-C20-C17	127.7(5)	C31-C30-C16	118.2(4)	C7-N1-C6	114.0(4)	C26-Fe1-C20	158.2(3)	C36-Fe2-C38	67.8(4)
N1-C6-C1	119.3(5)	C21-C20-C17	124.5(5)	C35-C31-C32	107.5(4)	C8-N2-C5	114.6(4)	C28-Fe1-C20	124.8(2)	C40-Fe2-C38	66.3(4)
N1-C6-C5	123.0(5)	C24-C20-Fe1	69.2(3)	C35-C31-C30	124.0(5)	C19-N3-C9	115.0(4)	C29-Fe1-C20	109.47(19)	C39-Fe2-C38	38.9(4)
C1-C6-C5	117.6(5)	C21-C20-Fe1	69.5(3)	C32-C31-C30	128.2(5)	C19-N3-C18	115.4(4)	C24-Fe1-C20	40.3(2)	C31-Fe2-C33	69.3(2)
N1-C7-C11	128.3(4)	C17-C20-Fe1	131.7(3)	C35-C31-Fe2	71.3(3)	C9-N3-C18	108.9(3)	C22-Fe1-C20	68.48(19)	C37-Fe2-C33	161.8(4)
N1-C7-C8	122.2(5)	C20-C21-C22	107.6(6)	C32-C31-Fe2	69.4(3)	C23-Fe1-C26	123.4(3)	C21-Fe1-C20	40.5(2)	C32-Fe2-C33	41.2(2)
C11-C7-C8	109.5(4)	C20-C21-Fe1	70.0(3)	C30-C31-Fe2	120.7(3)	C23-Fe1-C28	121.5(3)	C25-Fe1-C20	123.7(2)	C36-Fe2-C33	155.9(4)
N2-C8-C7	124.9(5)	C22-C21-Fe1	69.0(3)	C31-C32-C33	107.4(5)	C26-Fe1-C28	67.7(3)	C23-Fe1-C27	106.8(3)	C40-Fe2-C33	120.6(4)
N2-C8-C9	125.6(4)	C23-C22-C21	107.6(6)	C31-C32-Fe2	68.8(3)	C23-Fe1-C29	157.2(3)	C26-Fe1-C27	40.0(3)	C39-Fe2-C33	108.5(4)
C7-C8-C9	109.5(4)	C23-C22-Fe1	69.4(4)	C33-C32-Fe2	70.8(3)	C26-Fe1-C29	67.5(3)	C28-Fe1-C27	40.7(3)	C31-Fe2-C35	41.1(2)
N3-C9-C10	111.3(4)	C21-C22-Fe1	69.9(3)	C34-C33-C32	107.2(5)	C28-Fe1-C29	39.9(3)	C29-Fe1-C27	67.6(3)	C37-Fe2-C35	107.3(4)
N3-C9-C8	116.1(4)	C22-C23-C24	108.9(6)	C34-C33-Fe2	71.0(4)	C23-Fe1-C24	40.5(2)	C24-Fe1-C27	124.1(3)	C32-Fe2-C35	69.0(3)
C10-C9-C8	100.4(4)	C22-C23-Fe1	70.5(4)	C32-C33-Fe2	68.0(3)	C26-Fe1-C24	159.9(3)	C22-Fe1-C27	120.4(3)	C36-Fe2-C35	127.2(4)
N3-C9-C16	102.5(3)	C24-C23-Fe1	70.4(3)	C33-C34-C35	110.8(6)	C28-Fe1-C24	108.2(3)	C21-Fe1-C27	156.7(2)	C40-Fe2-C35	167.1(4)
C10-C9-C16	115.7(4)	C23-C24-C20	108.5(6)	C33-C34-Fe2	69.7(4)	C29-Fe1-C24	122.9(3)	C25-Fe1-C27	67.4(3)	C39-Fe2-C35	151.1(4)
C8-C9-C16	111.4(3)	C23-C24-Fe1	69.2(4)	C35-C34-Fe2	69.7(3)	C23-Fe1-C22	40.1(3)	C20-Fe1-C27	160.9(3)	C38-Fe2-C35	118.3(4)
C15-C10-C11	118.3(4)	C20-C24-Fe1	70.5(3)	C34-C35-C31	107.1(6)	C26-Fe1-C22	107.3(3)	C31-Fe2-C37	119.3(3)	C33-Fe2-C35	67.8(3)
C15-C10-C9	128.1(4)	C26-C25-C29	106.6(7)	C34-C35-Fe2	70.7(4)	C28-Fe1-C22	156.0(3)	C31-Fe2-C32	41.8(2)	C31-Fe2-C34	67.7(2)
C11-C10-C9	113.5(4)	C26-C25-Fe1	69.3(4)	C31-C35-Fe2	67.6(3)	C29-Fe1-C22	162.0(4)	C37-Fe2-C32	155.4(4)	C37-Fe2-C34	126.1(4)
C12-C11-C10	122.0(5)	C29-C25-Fe1	68.9(3)	C37-C36-C40	104.9(7)	C24-Fe1-C22	67.9(3)	C31-Fe2-C36	108.4(2)	C32-Fe2-C34	67.5(3)
C12-C11-C7	131.1(5)	C25-C26-C27	110.4(7)	C37-C36-Fe2	68.9(4)	C23-Fe1-C21	68.1(3)	C37-Fe2-C36	40.7(4)	C36-Fe2-C34	163.7(5)

C10-C11-C7	106.9(4)	C25-C26-Fe1	71.1(4)	C40-C36-Fe2	69.2(4)	C26-Fe1-C21	122.4(3)	C32-Fe2-C36	121.0(4)	C40-Fe2-C34	152.8(4)
C11-C12-C13	118.5(5)	C27-C26-Fe1	71.3(4)	C38-C37-C36	109.3(10)	C28-Fe1-C21	161.5(2)	C31-Fe2-C40	129.7(3)	C39-Fe2-C34	119.3(3)
C12-C13-C14	120.6(5)	C26-C27-C28	106.6(7)	C38-C37-Fe2	71.8(5)	C29-Fe1-C21	125.8(3)	C37-Fe2-C40	67.8(4)	C38-Fe2-C34	108.0(4)
C15-C14-C13	121.2(5)	C26-C27-Fe1	68.7(4)	C36-C37-Fe2	70.4(5)	C24-Fe1-C21	67.8(2)	C32-Fe2-C40	110.1(3)	C33-Fe2-C34	39.3(3)
C14-C15-C10	119.3(5)	C28-C27-Fe1	68.6(3)	C39-C38-C37	107.8(10)	C22-Fe1-C21	41.1(3)	C36-Fe2-C40	41.5(4)	C35-Fe2-C34	39.6(2)
C30-C16-C17	116.0(4)	C29-C28-C27	108.2(6)	C39-C38-Fe2	69.6(5)	C23-Fe1-C25	159.3(3)	C31-Fe2-C39	167.0(4)	-	-
C30-C16-C9	113.4(3)	C29-C28-Fe1	70.1(3)	C37-C38-Fe2	68.2(4)	C26-Fe1-C25	39.6(3)	C37-Fe2-C39	66.8(4)	-	-

Conclusion

The crystal structure analysis of two novel Ferrocene derivatives was studied using single crystal X-ray diffraction method. The packing of Ferr1 is stabilized by intermolecular C–H···O, C–H···S, intramolecular C–H···Cg, C–H···N hyrdrogen bonds, and the packing of Ferr2 is stabilized by intermolecular C–H···O and intramolecular C–H···Cg hydrogen bonds.

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