SUPPORTING INFORMATION FOR

"Novel Ferrocene Polyene Derivatives and Their Binding to Unmodified Cyclodextrins"

Jian Liu,[a] René Castro,[a] Khalil A. Abboud,[b] and Angel E. Kaifer*,[a]

[a]*Center for Supramolecular Science and Department of Chemistry, University of Miami, Coral Gables, FL 33124-0431, and*

[b]*Chemistry Department, University of Florida, Gainesville, FL 32611.*

Table S1. Crystal data and structure refinement for compound **1**.

Identification code	akf2	
Empirical formula	C17 H16 Fe O	
Formula weight	292.15	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 6.0990(1) Å	α= 90°.
	b = 7.5055(1) Å	β= 95.555(1)°.
	c = 14.6123(3) Å	γ = 90°.
Volume	665.71(2) $Å^3$	
Z	2	
Density (calculated)	1.457 Mg/m^3	
Absorption coefficient	1.120 mm^{-1}	
F(000)	304	
Crystal size	0.32 x 0.21 x 0.16 mm^3	
Theta range for data collection	1.40 to 27.50°.	
Index ranges	-4=h=8, -10=k=10, -19=l=18	
Reflections collected	4755	
Independent reflections	2952 [R(int) = 0.0193]	
Absorption correction	Empirical	
Max. and min. transmission	0.978 and 0.745	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2951 / 1 / 172	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0250, wR2 = 0.0641 [2839]	
R indices (all data)	R1 = 0.0266, wR2 = 0.0807	
Absolute structure parameter	0.039(15)	
Largest diff. peak and hole	0.313 and -0.427 e.$Å^{-3}$	

$R1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$

$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w= 1/[\sigma^2(F_o^2)+(0.0370*p)^2+0.31*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe	2672(1)	6448(1)	1459(1)	18(1)
O1	-8313(3)	5664(3)	7092(1)	49(1)
C1	2866(3)	5282(2)	2741(1)	21(1)
C2	2001(3)	4046(2)	2042(1)	21(1)
C3	3609(3)	3829(2)	1406(1)	23(1)
C4	5456(3)	4916(3)	1692(1)	24(1)
C5	5010(3)	5838(3)	2510(1)	22(1)
C1'	30(4)	8147(3)	1277(2)	31(1)
C2'	174(4)	7110(3)	476(2)	31(1)
C3'	2226(4)	7437(3)	148(2)	36(1)
C4'	3376(4)	8685(3)	743(2)	41(1)
C5'	1988(5)	9125(3)	1448(2)	36(1)
C6	1832(3)	5905(3)	3534(1)	23(1)
C7	-8(3)	5204(3)	3833(1)	23(1)
C8	-955(3)	5831(3)	4640(1)	23(1)
C9	-2834(3)	5172(3)	4929(1)	24(1)
C10	-3758(3)	5799(3)	5739(1)	24(1)
C11	-5695(4)	5236(3)	6018(1)	25(1)
C12	-6536(4)	6004(3)	6822(1)	31(1)

Table S3. Bond lengths [Å] and angles [°] for compound **1**.

Fe-C5	2.044(2)
Fe-C4'	2.046(2)
Fe-C3'	2.048(2)
Fe-C3	2.050(2)
Fe-C2'	2.051(2)
Fe-C4	2.051(2)
Fe-C2	2.052(2)
Fe-C5'	2.052(2)
Fe-C1'	2.052(2)
Fe-C1	2.060(2)
O1-C12	1.216(3)
C1-C2	1.441(3)
C1-C5	1.443(3)
C1-C6	1.450(3)
C2-C3	1.425(3)
C2-H2	1.00
C3-C4	1.420(3)
C3-H3	1.00
C4-C5	1.430(3)
C4-H4	1.00
C5-H5	1.00
C1'-C5'	1.403(4)
C1'-C2'	1.415(3)
C1'-H1'	1.00
C2'-C3'	1.404(3)
C2'-H2'	1.00
C3'-C4'	1.417(4)
C3'-H3'	1.00
C4'-C5'	1.434(4)
C4'-H4'	1.00
C5'-H5'	1.00
C6-C7	1.349(3)
C6-H6	0.95
C7-C8	1.441(3)

C7-H7	0.95
C8-C9	1.352(3)
C8-H8	0.95
C9-C10	1.438(3)
C9-H9	0.95
C10-C11	1.354(3)
C10-H10	0.95
C11-C12	1.447(3)
C11-H11	0.95
C12-H12	0.95

C5-Fe-C4'	113.71(9)
C5-Fe-C3'	143.51(10)
C4'-Fe-C3'	40.50(11)
C5-Fe-C3	68.73(8)
C4'-Fe-C3	133.97(10)
C3'-Fe-C3	108.93(9)
C5-Fe-C2'	175.76(9)
C4'-Fe-C2'	67.76(10)
C3'-Fe-C2'	40.07(10)
C3-Fe-C2'	113.38(8)
C5-Fe-C4	40.89(8)
C4'-Fe-C4	109.47(9)
C3'-Fe-C4	113.03(9)
C3-Fe-C4	40.52(8)
C2'-Fe-C4	143.01(9)
C5-Fe-C2	69.15(8)
C4'-Fe-C2	173.51(11)
C3'-Fe-C2	133.89(9)
C3-Fe-C2	40.65(8)
C2'-Fe-C2	109.84(8)
C4-Fe-C2	68.54(8)
C5-Fe-C5'	110.59(9)
C4'-Fe-C5'	40.96(11)
C3'-Fe-C5'	68.22(9)
C3-Fe-C5'	174.60(11)

C2'-Fe-C5'	67.68(9)
C4-Fe-C5'	135.60(10)
C2-Fe-C5'	144.57(10)
C5-Fe-C1'	135.93(9)
C4'-Fe-C1'	67.95(10)
C3'-Fe-C1'	67.77(9)
C3-Fe-C1'	144.02(9)
C2'-Fe-C1'	40.34(9)
C4-Fe-C1'	175.36(9)
C2-Fe-C1'	114.47(9)
C5'-Fe-C1'	39.98(10)
C5-Fe-C1	41.17(8)
C4'-Fe-C1	144.77(10)
C3'-Fe-C1	174.31(10)
C3-Fe-C1	68.64(8)
C2'-Fe-C1	135.47(9)
C4-Fe-C1	68.75(8)
C2-Fe-C1	41.03(8)
C5'-Fe-C1	114.63(8)
C1'-Fe-C1	110.93(8)
C2-C1-C5	107.4(2)
C2-C1-C6	128.0(2)
C5-C1-C6	124.6(2)
C2-C1-Fe	69.17(10)
C5-C1-Fe	68.80(11)
C6-C1-Fe	126.78(13)
C3-C2-C1	107.9(2)
C3-C2-Fe	69.61(10)
C1-C2-Fe	69.80(10)
C3-C2-H2	126.04(11)
C1-C2-H2	126.04(11)
Fe-C2-H2	126.04(5)
C4-C3-C2	108.6(2)
C4-C3-Fe	69.77(11)
C2-C3-Fe	69.74(10)
C4-C3-H3	125.70(11)

C2-C3-H3	125.70(11)
Fe-C3-H3	125.70(5)
C3-C4-C5	108.3(2)
C3-C4-Fe	69.71(11)
C5-C4-Fe	69.28(11)
C3-C4-H4	125.84(11)
C5-C4-H4	125.84(11)
Fe-C4-H4	125.84(6)
C4-C5-C1	107.8(2)
C4-C5-Fe	69.83(11)
C1-C5-Fe	70.03(11)
C4-C5-H5	126.11(11)
C1-C5-H5	126.11(11)
Fe-C5-H5	126.11(5)
C5'-C1'-C2'	108.4(2)
C5'-C1'-Fe	70.00(13)
C2'-C1'-Fe	69.78(12)
C5'-C1'-H1'	125.82(14)
C2'-C1'-H1'	125.82(13)
Fe-C1'-H1'	125.82(6)
C3'-C2'-C1'	108.4(2)
C3'-C2'-Fe	69.86(13)
C1'-C2'-Fe	69.88(12)
C3'-C2'-H2'	125.81(14)
C1'-C2'-H2'	125.81(13)
Fe-C2'-H2'	125.81(6)
C2'-C3'-C4'	108.1(2)
C2'-C3'-Fe	70.07(12)
C4'-C3'-Fe	69.64(13)
C2'-C3'-H3'	125.97(14)
C4'-C3'-H3'	125.97(15)
Fe-C3'-H3'	125.97(7)
C3'-C4'-C5'	107.5(2)
C3'-C4'-Fe	69.85(13)
C5'-C4'-Fe	69.76(12)
C3'-C4'-H4'	126.23(15)

C5'-C4'-H4'	126.23(15)
Fe-C4'-H4'	126.23(7)
C1'-C5'-C4'	107.7(2)
C1'-C5'-Fe	70.02(13)
C4'-C5'-Fe	69.28(13)
C1'-C5'-H5'	126.17(14)
C4'-C5'-H5'	126.17(15)
Fe-C5'-H5'	126.17(6)
C7-C6-C1	124.9(2)
C7-C6-H6	117.53(11)
C1-C6-H6	117.53(11)
C6-C7-C8	123.3(2)
C6-C7-H7	118.35(11)
C8-C7-H7	118.35(11)
C9-C8-C7	123.7(2)
C9-C8-H8	118.14(12)
C7-C8-H8	118.14(11)
C8-C9-C10	123.3(2)
C8-C9-H9	118.36(12)
C10-C9-H9	118.36(12)
C11-C10-C9	124.7(2)
C11-C10-H10	117.67(12)
C9-C10-H10	117.67(12)
C10-C11-C12	120.6(2)
C10-C11-H11	119.71(12)
C12-C11-H11	119.71(12)
O1-C12-C11	125.2(2)
O1-C12-H12	117.39(14)
C11-C12-H12	117.39(12)

Symmetry transformations used to generate equivalent atoms.

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe	21(1)	15(1)	18(1)	1(1)	0(1)	0(1)
O1	46(1)	56(1)	51(1)	3(1)	25(1)	0(1)
C1	24(1)	20(1)	18(1)	3(1)	0(1)	1(1)
C2	25(1)	16(1)	23(1)	2(1)	-1(1)	-2(1)
C3	30(1)	15(1)	24(1)	0(1)	0(1)	3(1)
C4	23(1)	23(1)	26(1)	2(1)	2(1)	2(1)
C5	22(1)	22(1)	22(1)	0(1)	-4(1)	0(1)
C1'	33(1)	29(1)	31(1)	7(1)	4(1)	11(1)
C2'	37(1)	27(1)	27(1)	4(1)	-12(1)	0(1)
C3'	56(2)	32(1)	22(1)	12(1)	10(1)	13(1)
C4'	33(1)	32(1)	59(2)	28(1)	4(1)	-2(1)
C5'	56(2)	15(1)	35(1)	1(1)	-11(1)	2(1)
C6	29(1)	20(1)	19(1)	-1(1)	-1(1)	1(1)
C7	29(1)	21(1)	20(1)	1(1)	0(1)	1(1)
C8	29(1)	20(1)	21(1)	1(1)	-1(1)	3(1)
C9	30(1)	21(1)	21(1)	0(1)	1(1)	1(1)
C10	29(1)	19(1)	23(1)	1(1)	-1(1)	2(1)
C11	30(1)	23(1)	24(1)	1(1)	1(1)	-1(1)
C12	39(1)	27(1)	27(1)	2(1)	7(1)	2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **1**.

	x	y	z	U(eq)
H2	530(3)	3448(2)	2009(1)	26
H3	3454(3)	3055(2)	846(1)	28
H4	6821(3)	5035(3)	1369(1)	29
H5	6012(3)	6703(3)	2863(1)	27
H1'	-1247(4)	8176(3)	1657(2)	37
H2'	-985(4)	6282(3)	194(2)	37
H3'	2777(4)	6887(3)	-410(2)	43
H4'	4877(4)	9178(3)	680(2)	49
H5'	2348(5)	9976(3)	1967(2)	44
H6	2499(3)	6880(3)	3869(1)	27
H7	-714(3)	4249(3)	3494(1)	28
H8	-219(3)	6759(3)	4988(1)	28
H9	-3580(3)	4249(3)	4580(1)	29
H10	-2952(3)	6670(3)	6104(1)	29
H11	-6508(4)	4328(3)	5683(1)	31
H12	-5626(4)	6841(3)	7167(1)	37

Figure Captions

Figure SI1. Thermal ellipsoids drawing of compound **1** with 50% probability ellipsoids and the atomic numbering scheme.

Figure SI2. Packing diagram (viewed from axis *a*) for the crystal structure of compound **1**.

Fig. S1

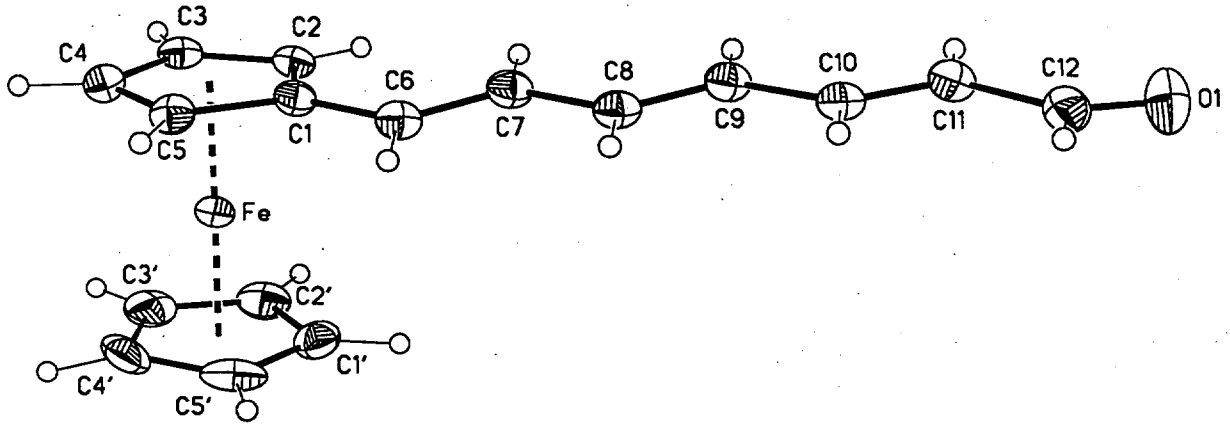

Fig. S2