Supporting Information

Control of the Reversibility During Boronic Etser Formation: Application to the Construction of Ferrocene Dimers and Trimers

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NMR spectra of *homo*-3

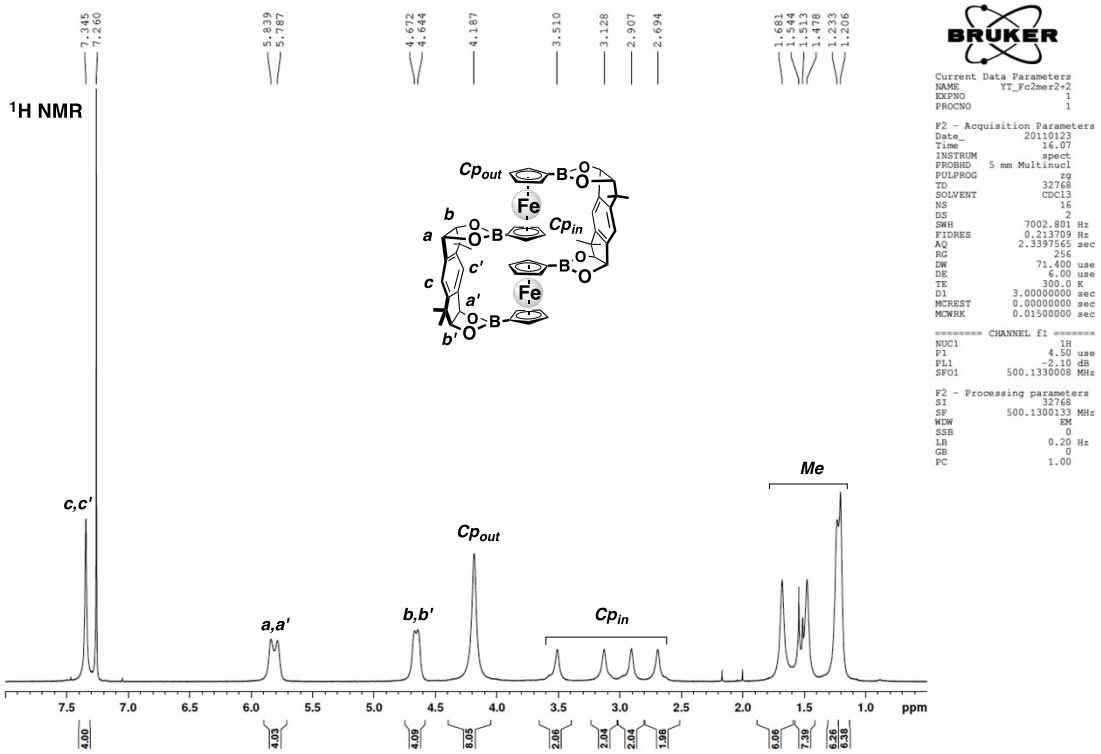


Fig. S1 ^{1}H NMR (500 MHz, $CDCl_3$, 300 K) spectrum of *homo*-**3**.

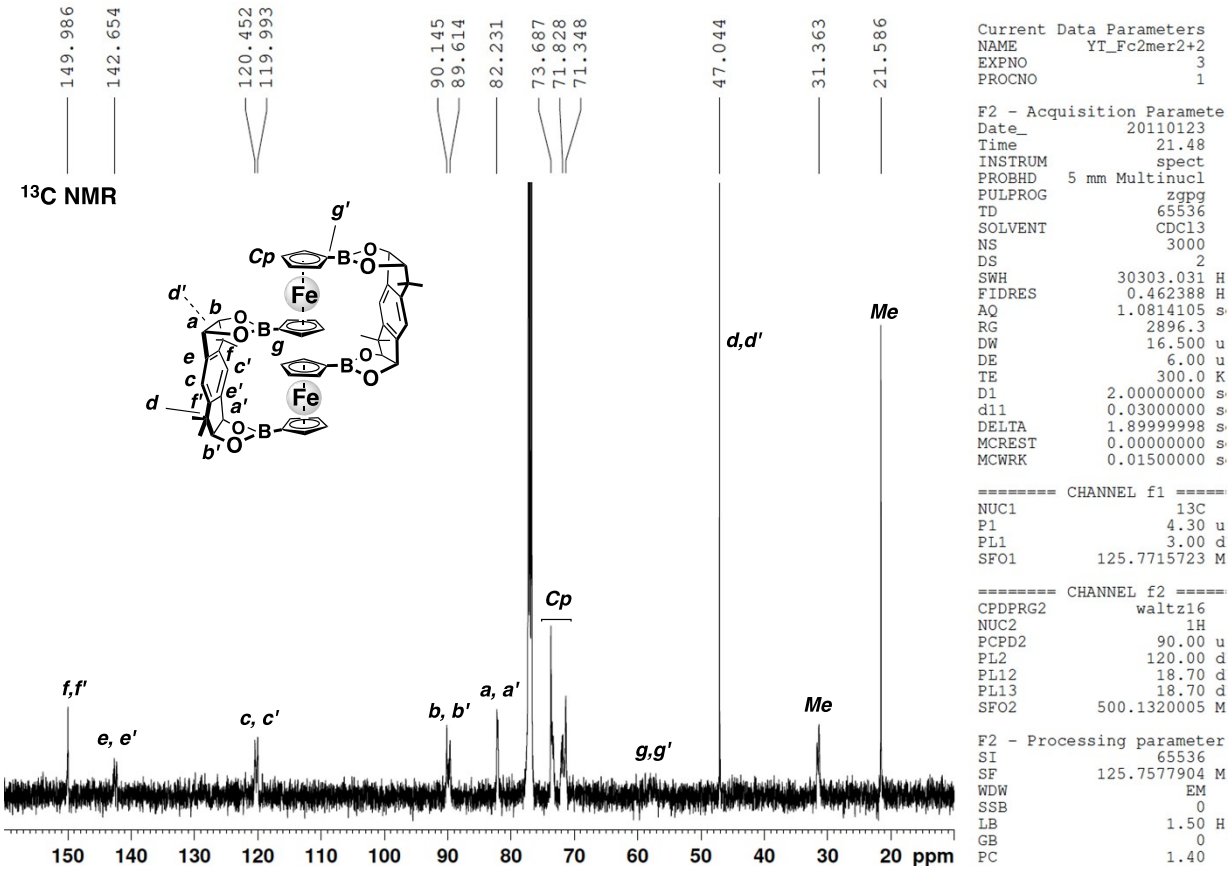


Fig. S2 ^{13}C NMR (125 MHz, $CDCl_3$, 300 K) spectrum of *homo*-**3**.

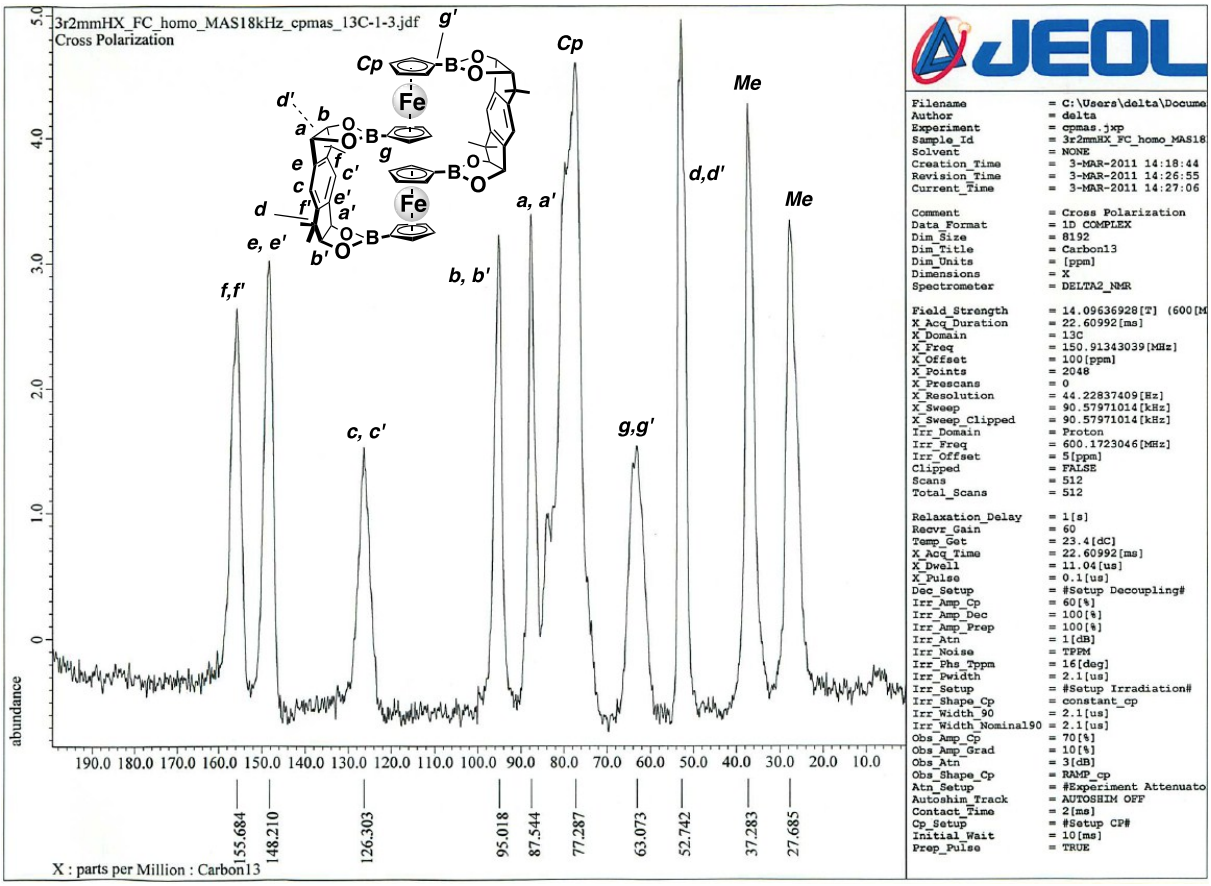


Fig. S3 CPMAS ^{13}C NMR (150 MHz, 296 K) spectrum of *homo*-**3**.

NMR spectra of *hetero*-3

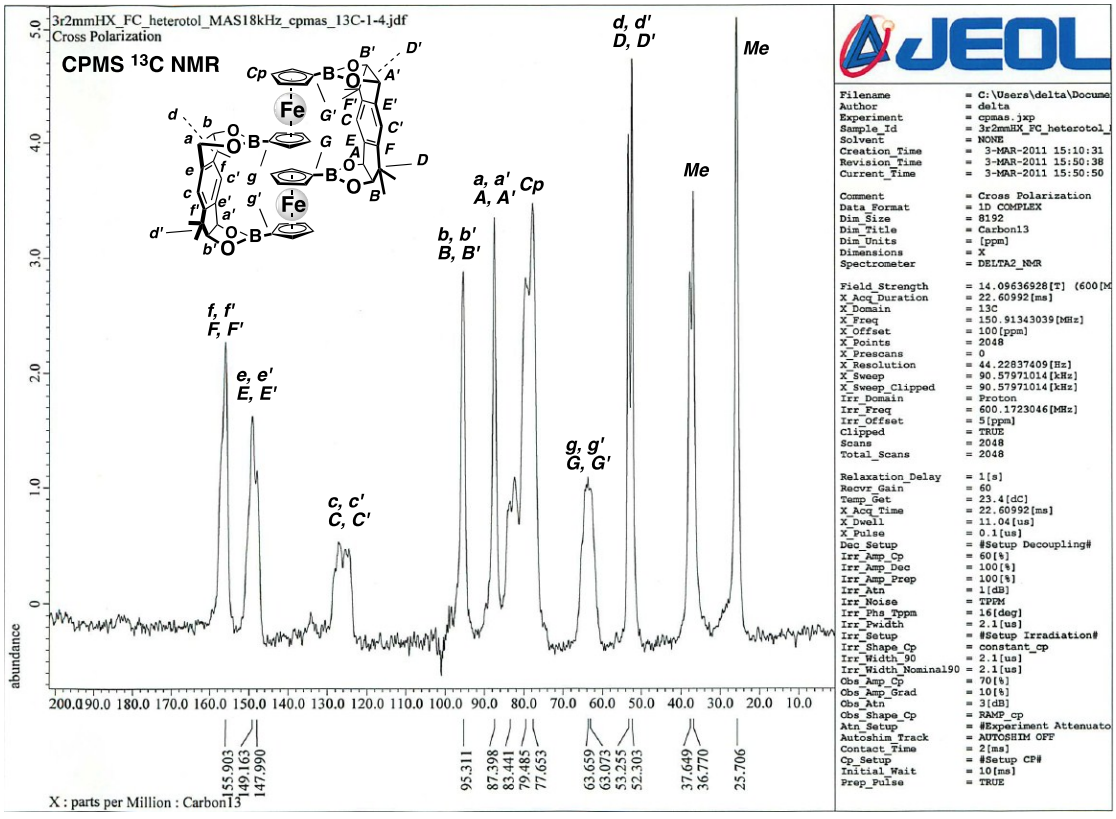
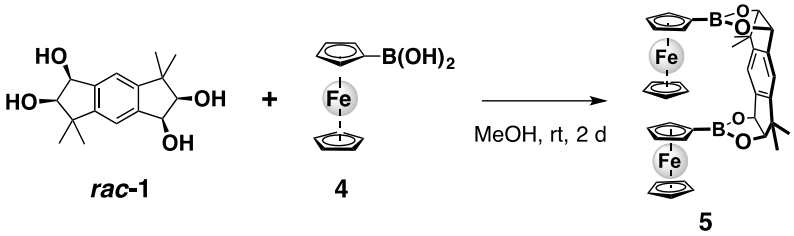


Fig. S4 CPMAS ^{13}C NMR (150 MHz, 296 K) spectrum of *hetero*-**3**.

Synthesis of 5



Ferroceneboronic acid **4** (18.3 mg, 0.080 mmol) was added to a methanol solution (3.2 mL) of tetrol **1** (11.1 mg, 0.040 mmol). The reaction mixture became homogeneous in a moment, and in a few minutes precipitation started to appear. After the mixture was stirred at room temperature for 2 days, **5** (20.5 mg, 77%) was obtained as an orange powder by filtration.

Physical data of 5

^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 7.40 (s, 2H), 5.81 (d, J = 5.8 Hz, 2H), 4.77 (d, J = 5.8 Hz, 2H), 4.30 (br, 2H), 4.29 (br, 2H), 4.27 (br, 4H), 3.79 (s, 10H), 1.47 (s, 6H), 1.31 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$, 300 K): δ = 150.2 (C_q), 141.7 (C_q), 120.5 (*C*H), 90.0 (*C*H), 82.6 (*C*H), 73.7 (*C*H), 73.4 (*C*H), 71.9 (*C*H), 71.9 (*C*H), 68.3 (*C*H), 57.7 (C_q), 46.6 (C_q), 30.9 (CH_3), 23.4 (CH_3).

HRMS (FD$^+$): *m/z* Calcd. for $C_{36}H_{36}B_2Fe_2O_4$: 666.15028, Found: 666.14985 $[M]^+$.

IR (KBr): 2955, 2932, 1499, 1484, 1383, 1365, 1316, 1301, 1217, 1183, 1126 cm^{-1}.

m.p.: 227 ºC (decomposed).

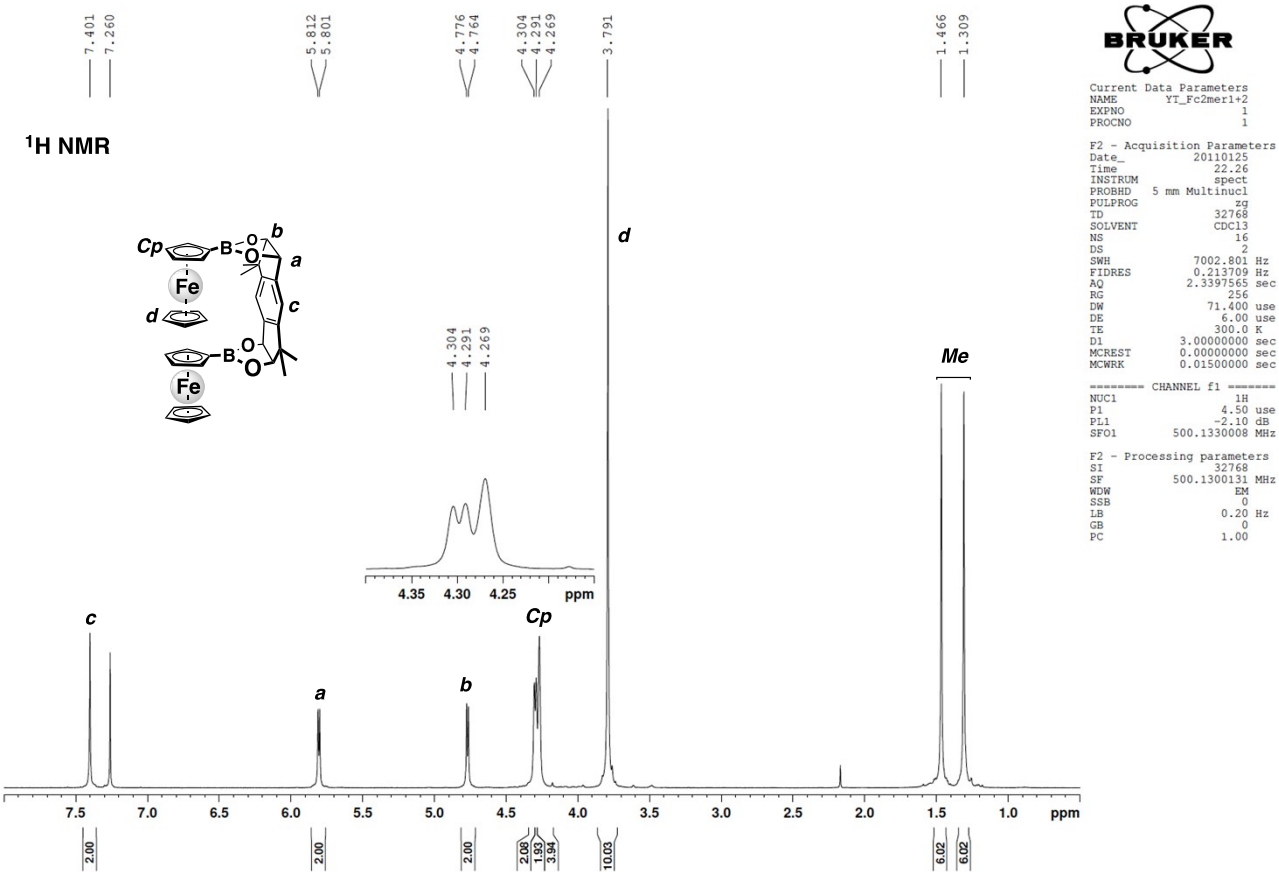


Fig. S5 ^{1}H NMR (500 MHz, $CDCl_3$, 300 K) spectrum of **5**.

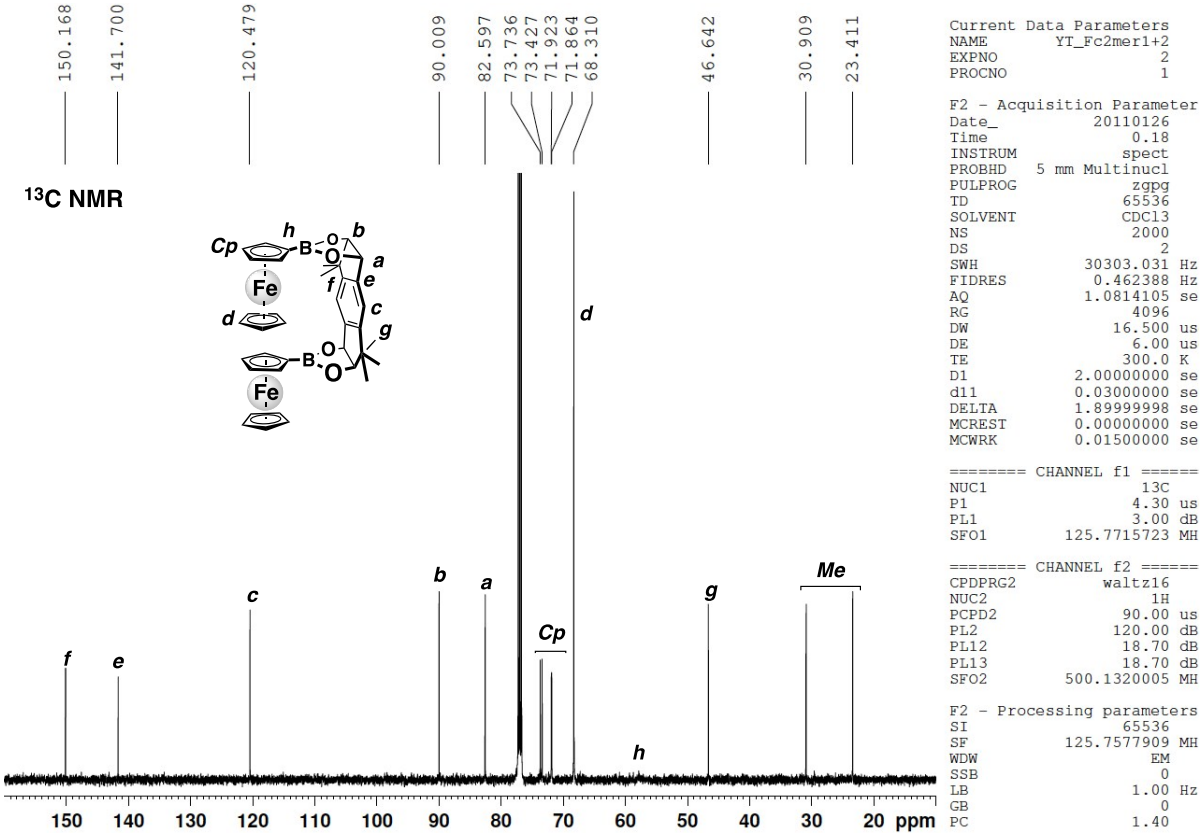
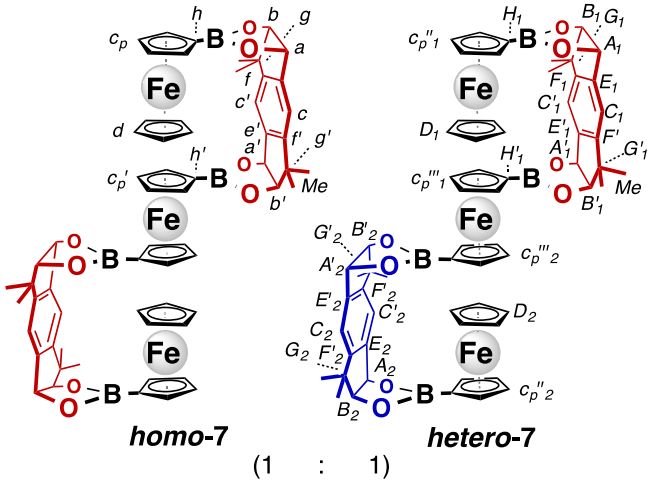


Fig. S6 ^{13}C NMR (125 MHz, $CDCl_3$, 300 K) spectrum of **5**.

NMR spectra of trimer 7

Trimer 7 is composed of an equimolar amount of *homo*-**7** and *hetero*-**7**.



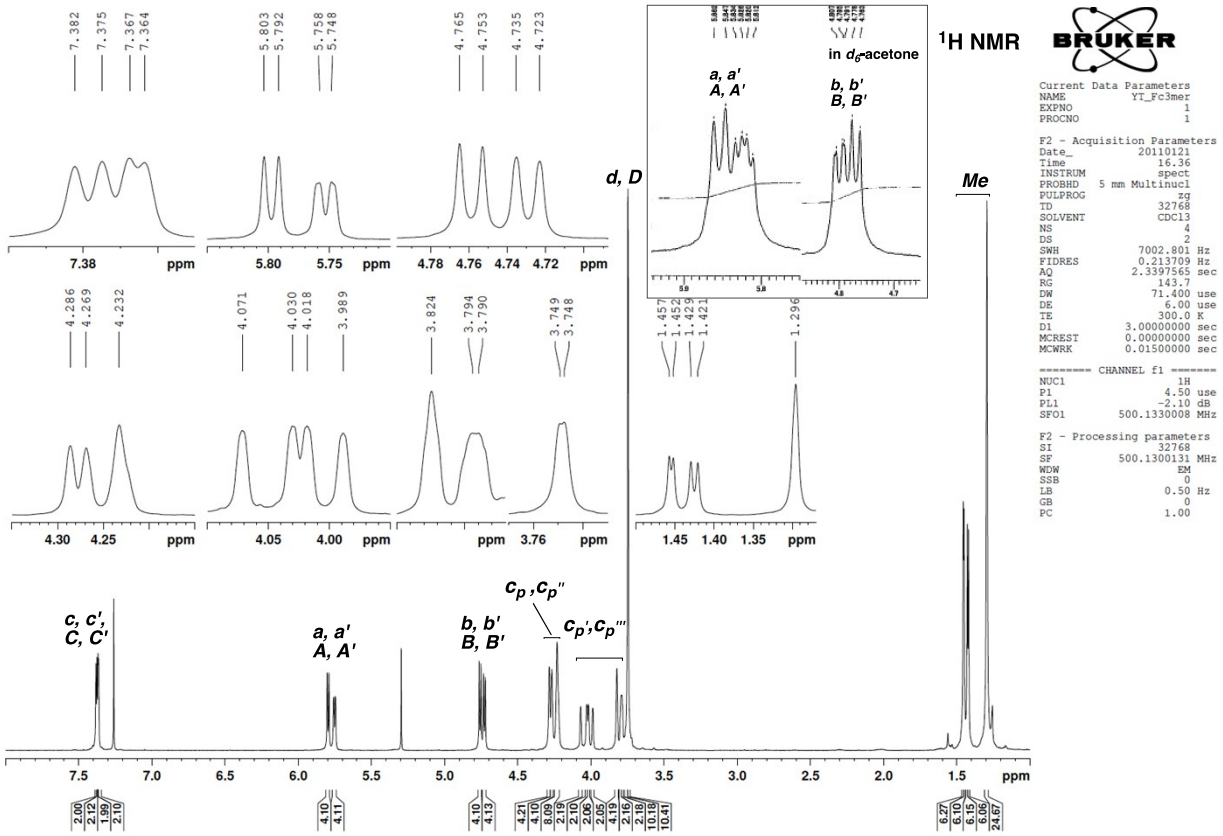


Fig. S7 ^{1}H NMR (500 MHz, $CDCl_3$, 300 K) spectrum of trimer **7** and extended ^{1}H NMR spectra of (*a, a', A, A'*) and (*b, b', B, B'*) regions in d_6-acteone in the inset.

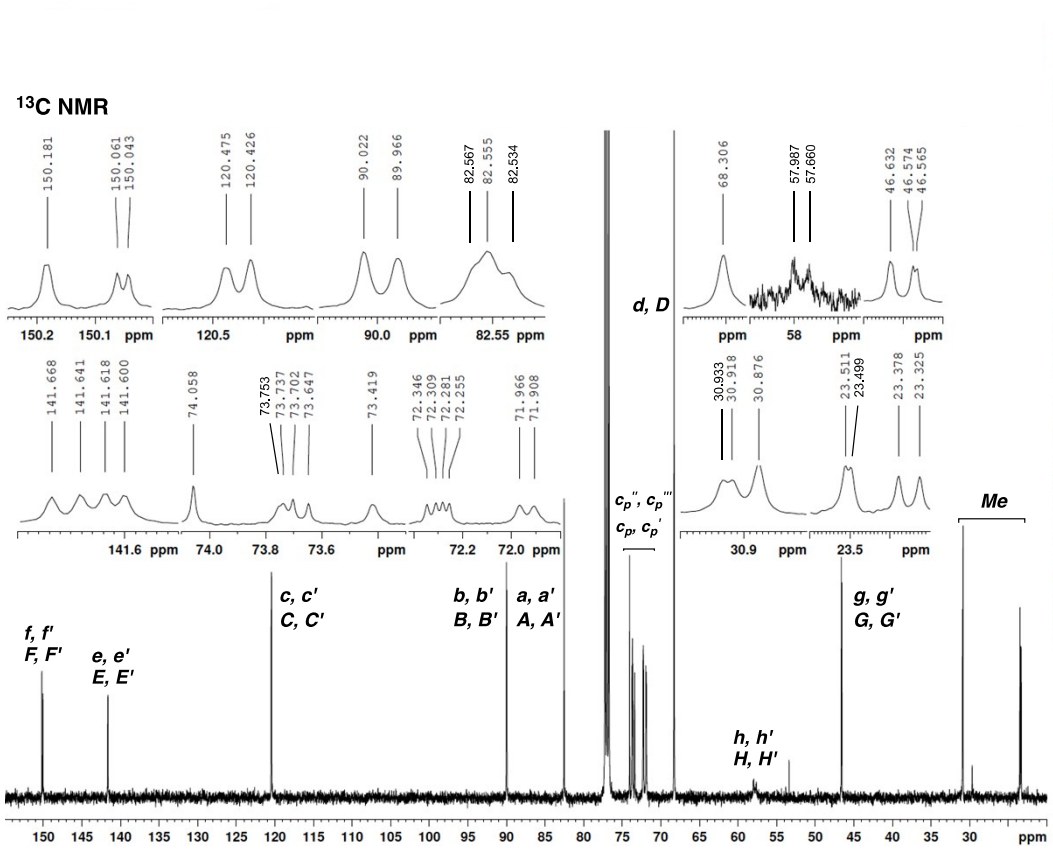


Fig. S8 ^{13}C NMR (125 MHz, $CDCl_3$, 300 K) spectrum of trimer **7**.

Physical data of tetramer

^{1}H NMR (500 MHz, $CDCl_3$, 300 K): δ = 7.39 ~ 7.37 (4H), 7.35 ~ 7.33 (2H), 5.80 (d, J = 6.0 Hz, 2H), 5.77 ~ 5.74 (4H), 4.75 (d, J = 6.0 Hz, 2H), 4.73 ~ 4.72 (4H), 4.27 ~ 4.25 (4H), 4.21 (br, 4H), 4.08 ~ 3.99 (8H), 3.84 ~ 3.78 (8H), 3.72 (s, 10H), 1.46 ~ 1.39 (18H), 1.29 (s, 18H).

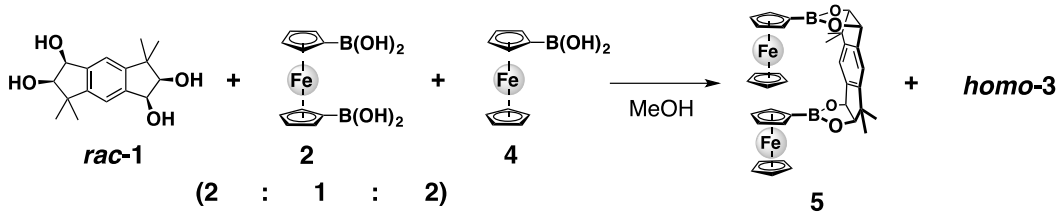
^{13}C NMR (125 MHz, $CDCl_3$, 300 K): δ = 150.2 (C_q), 150.1 (C_q), 150.1 (C_q), 141.7 (C_q), 141.7 (C_q), 141.6 (C_q), 141.5 (C_q), 141.5 (C_q), 141.5 (C_q), 120.5 (*C*H), 120.4 (*C*H), 90.0 (*C*H), 90.0 (*C*H), 90.0 (*C*H), 82.6 (*C*H), 74.1 (*C*H), 74.1 (*C*H), 73.7 (*C*H), 73.7 (*C*H), 73.4 (*C*H), 72.4 (*C*H), 72.3 (*C*H), 72.3 (*C*H), 72.0 (*C*H), 68.3 (*C*H), 58.1 (C_q), 46.6 (C_q), 46.6 (C_q), 46.5 (C_q), 30.9 (CH_3), 30.9 (CH_3), 23.6 (CH_3), 23.5 (CH_3), 23.5 (CH_3), 23.3 (CH_3), 23.3 (CH_3).

HRMS (FAB$^+$, NBA): *m/z* Calcd. for $C_{88}H_{89}B_6Fe_4O_{12}$: 1627.4270, Found: 1627.4282 $[M+H]^+$.

IR (KBr): 2956, 2926, 2365, 1480, 1382, 1315, 1298, 1214, 1180, 1125 cm^{-1}.

m.p.: 170 ºC.

Examination for construction of trimer 7 in MeOH under equilibrating conditions



All components, racemic tetrol **1** (13.8 mg, 0.050 mmol), 1,1'-ferrocenediboronic acid **2** (6.8 mg, 0.025 mmol), and ferroceneboronic acid **4** (11.4 mg, 0.050 mmol) (2 : 1 : 2 ratio) for trimer **7** were mixed at a time in methanol (4 ml) and the mixture was further stirred for 1 day. The resulting orange precipitate was obtained by filtration. The filtrate contained **5** (NMR yield: 16%) and **6** (NMR yield: 12%) and the precipitate was dissolved in chloroform, filtered, and evaporated in vacuo to give an orange solid (18.1 mg) composed of *homo*-**3** (NMR yield: 32%) and **5** (NMR yield: 32%). NMR yields were based on tetrol **1**.

^{11}B NMR analysis of an acetone-d_6 or acetone-d_6/methanol-d_4 (9:1) solution of the mixture of *rac*-1, 2 and 4 (2:1:2)

rac-**1** (2.0 mg, 7.2 μmol), 1,1'-ferrocenediboronic acid **2** (1.0 mg, 3.7 μmol), and ferroceneboronic acid **4** (1.7 mg, 7.4 μmol) (2 : 1 : 2 ratio) for trimer **7** were mixed with anhydrous $MgSO_4$ (1.8 mg) at a time in acetone-d_6 (0.5 ml) or acetone-d_6/methanol-d_4 (0.45 ml/0.05 ml, 9:1). After these mixtures were further stirred for 1 day at room temperature, ^{11}B NMR was measured.

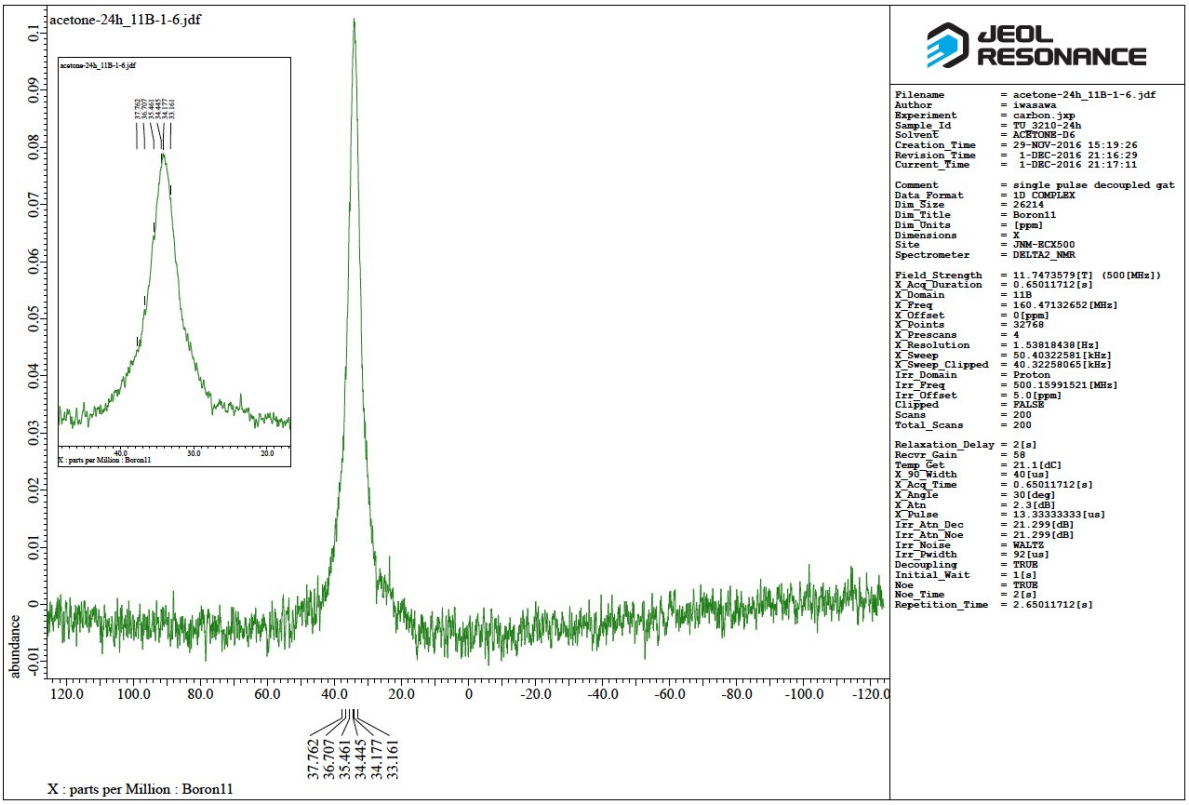


Fig. S9 ^{11}B NMR (160 MHz, acetone-d_6, 300 K) spectrum of the mixture of *rac*-**1**, **2** and **4** (2:1:2).

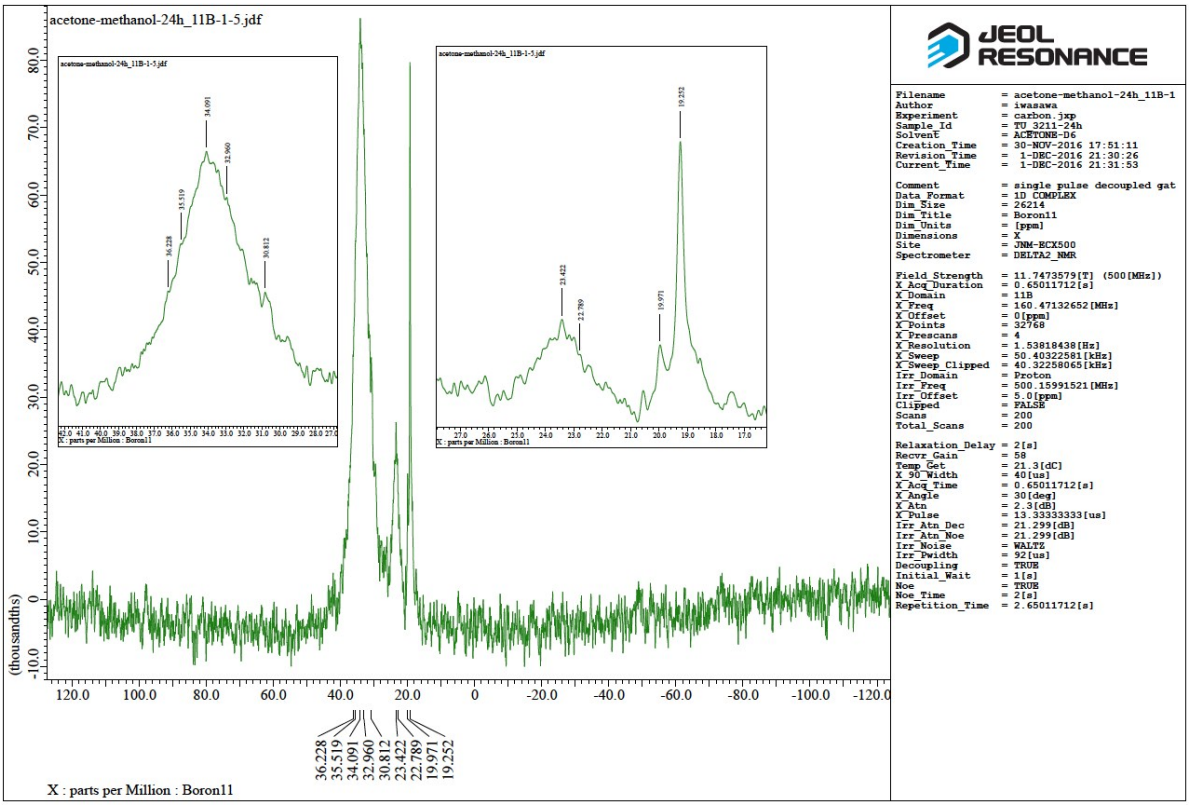


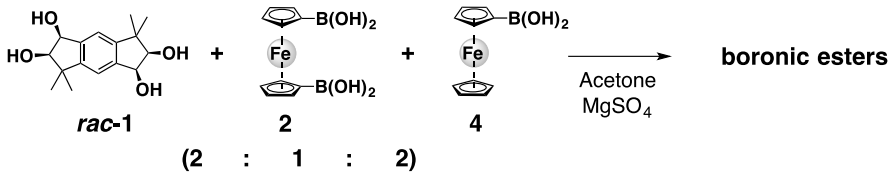
Fig. S10 ^{11}B NMR (160 MHz, acetone-d_6/methanol-d_4 (9:1), 300 K) spectrum of the mixture of *rac*-**1**, **2** and **4** (2:1:2).

In ^{11}B NMR of an acetone-d_6 solution of the mixture of *rac*-**1**, **2** and **4** (2:1:2) with anhydrous $MgSO_4$, one broad signal was observed at 34 ppm, suggesting only neutral boronate was present. On the other hand, in an acetone-d_6/methanol-d_4 (9:1) solution of the same mixture, besides broad signal at 34 ppm, up-field shifted signals at 23 and 19 ppm, which could be attributed to borate species were observed. Although exact assignment of these signals is not possible, this result might support that the addition of methanol generated the borate species and promoted the equilibration of boronic esters.

Examination for preparation of 6 in MeOH under equilibrating conditions

Ferroceneboronic acid **4** (34.4 mg, 0.150 mmol) was added to a methanol solution (13.2 mL) of tetrol **1** (41.6 mg, 0.150 mmol). The reaction mixture became homogeneous in a moment, and in a few minutes precipitation started to occur. After the mixture was stirred at room temperature for 1 day, **5** (37.0 mg, 37%) was obtained as an orange powder by filtration. The filtrate contained **6** (NMR yield: 20%), **5** (NMR yield: 7%) and tetrol (NMR yield: 36%). NMR yields were based on tetrol **1**.

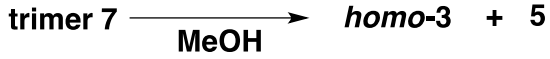
Examination for the one-pot construction of trimer 7 in acetone



All components, racemic tetrol **1** (13.8 mg, 0.050 mmol), 1,1'-ferrocenediboronic acid **2** (6.8 mg, 0.025 mmol), and ferroceneboronic acid **4** (11.4 mg, 0.050 mmol) (2 : 1 : 2 ratio) for trimer **7** were mixed at a time in acetone (4 ml) with anhydrous magnesium sulfate and the mixture was further stirred for 1 day. After removing the magnesium sulfate by filtration, the filtrate was concentrated and an orange solid was obtained (26.8 mg). Some insoluble orange materials remained over the surface of magnesium sulfate. The resulting crude product was purified by GPC to give trimer **7** (7.2 mg, 25%), **4-mer** (2.2 mg, 8%), ***homo*-3** (2.4 mg, 10%) and **5** (10.0 mg, 30%). Yields are based on tetrol **1**.

Although further analysis of insoluble materials was not carried out, ***hetero*-3** was also likely to be produced as some insoluble orange materials remained over the surface of magnesium sulfate and the recovery of tetrol **1** in the filtrate was small. In the stepwise assembly of trimer **7** (Fig. 3B), no obvious formation of ***homo*-3** or ***hetero*-3** was observed. This could be attributed to the amount of tetrol **1** present in the reaction mixture when ferrocenediboronic acid **2** was added (in the stepwise reaction, the amount of tetrol **1** remained was estimated to be 22%). We think by suppressing the generation of ***homo*-3** and/or ***hetero*-3**, somewhat higher yield (31%) of the target product trimer **7** was achieved.

Transformation of trimer 7 into *homo*-3 and 5 in MeOH under equilibrating conditions



Trimer **7** (7.5 mg, 6.5×10^{-3} mmol) was suspended in methanol (2 ml) for 12 h. The resulting orange precipitate was obtained by filtration. The precipitate was dissolved in chloroform, filtered, and evaporated in vacuo to give an orange solid (6.6 mg) composed of *homo*-**3** (NMR yield: 44%) and **5** (NMR yield: 43%). NMR yields were based on tetrol **1**.

Time-dependent behavior of trimer 7 in acetone-d_6 or acetone-d_6/CD_3OD-d_4 (=10:1)

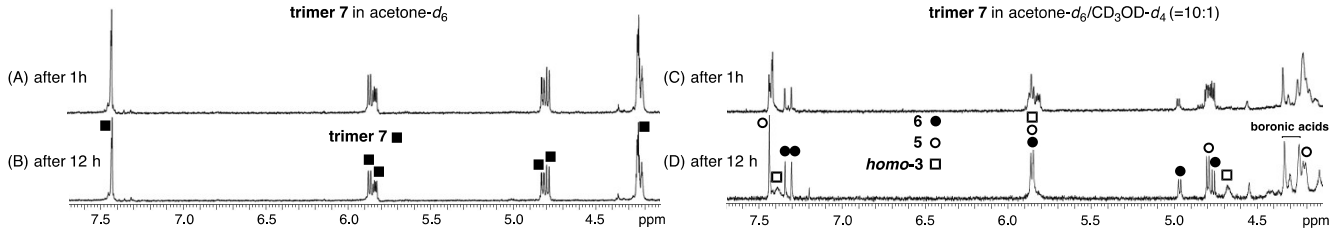


Fig. S11 Partial time-dependent ^{1}H NMR (400 MHz, 300 K) spectra of an acetone-d_6 solution of **7** (A, B) and an acetone-d_6/CD_3OD-d_4 (=10:1) solution of **7** (C, D).

An acetone-d_6 solution of trimer **7** and an acetone-d_6/CD_3OD-d_4 (=10:1) solution of **7** were prepared. From the time-dependent ^{1}H NMR study of these solutions, it was revealed that **7** was stable in acetone-d_6 after 12 h at r.t., however, transformation of **7** into **6**, **5, *homo*-3** or precipitate was observed in acetone-d_6/CD_3OD (=10:1) after 12 h at r.t.

Cyclic and differential pulse voltammograms of ferrocene oligomers

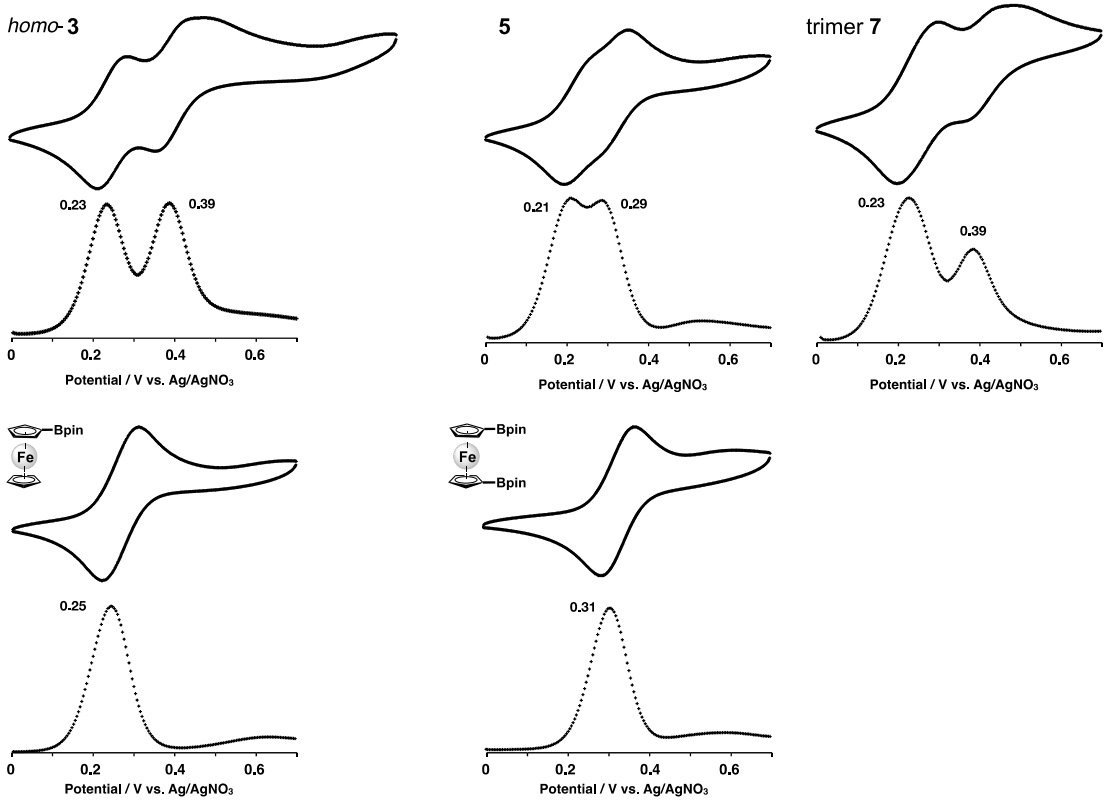


Fig. S12 Cyclic voltammograms (top view) and differential pulse voltammograms (bottom row) of *homo*-**3**, **5**, **7** and pinacolato esters of **4** and **2**.

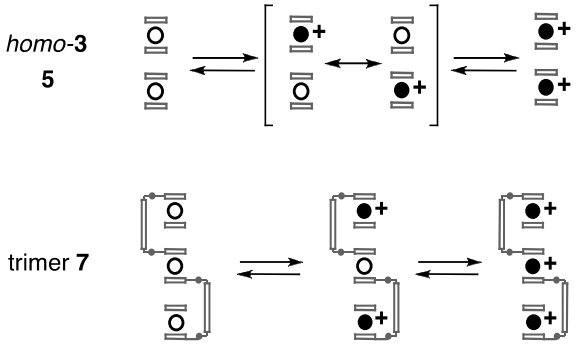


Fig. S13 A graphical representation of the electrochemical behavior of the *homo*-**3**, **5**, and **7**.

ORTEP drawing of *homo*-3•2$CHCl_3$

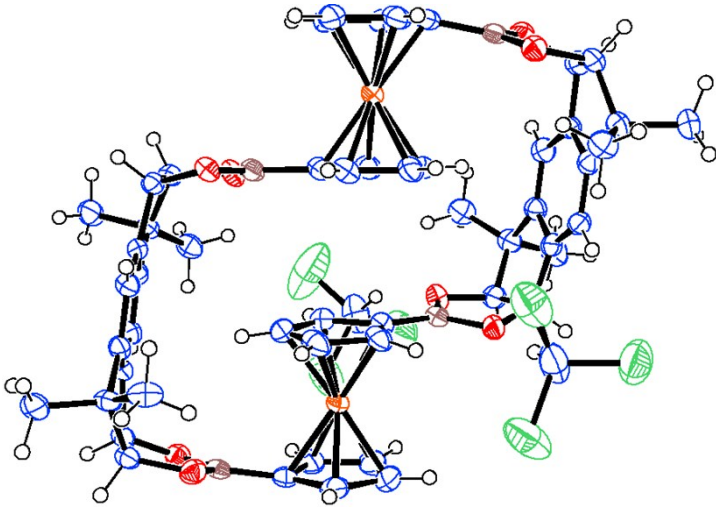


Fig. S14 ORTEP drawing (50% probability ellipsoids) of *homo*-**3**•2$CHCl_3$.

Table S1 Crystal data and structure refinement for *homo*-**3**•2$CHCl_3$.

Identification code	shelx	
Empirical formula	C_{54} H_{54} B_4 Cl_6 Fe_2 O_8	
Formula weight	1198.61	
Temperature	171(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 11.5229(6) Å	α = 65.367(1) °.
	b = 14.4999(8) Å	β = 70.676(2) °.
	c = 18.9095(11) Å	γ = 83.183(2) °.
Volume	2709.4(3) $Å^3$	
Z	2	
Density (calculated)	1.469 Mg/m^3	
Absorption coefficient	0.885 mm^{-1}	
F(000)	1232	
Crystal size	0.12 × 0.10 × 0.10 mm^3	
Theta range for data collection	3.09 to 27.45 °.	
Index ranges	–14<=h<=14, –18<=k<=18, –24<=l<=24	
Reflections collected	27014	
Independent reflections	12297 [R(int) = 0.0457]	
Completeness to theta = 27.45 °	99.2%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9167 and 0.9028	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12297 / 0 / 732	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1646	
R indices (all data)	R1 = 0.0839, wR2 = 0.1800	
Largest diff. peak and hole	1.959 and –1.228 e.$Å^{-3}$	
CCDC reference number	869450	

Crystal structure of *hetero*-3

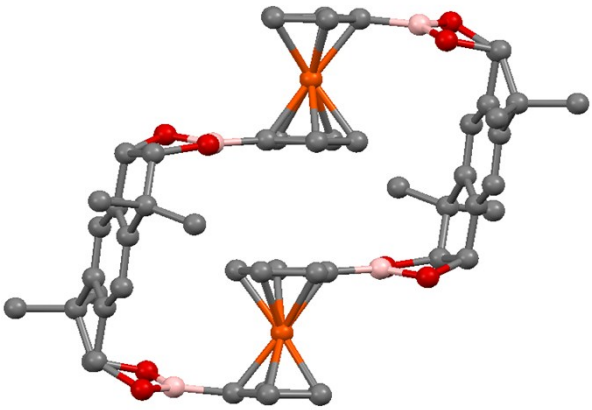


Fig. S15 Crystal structure of *hetero*-**3**.

Table S2 Crystal data and structure refinement for *hetero*-**3**.

Identification code	shelx	
Empirical formula	$C_{52}\ H_{52}\ B_4\ Fe_2\ O_8$	
Formula weight	959.88	
Temperature	293(2) K	
Wavelength	1.54186 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.6429(5) Å	α = 100.4774(35) °
	b = 15.1158(10) Å	β = 99.7785(18) °
	c = 7.5906(4) Å	γ = 107.4466(20) °
Volume	1112.30(14) Å^3	
Z	1	
Density (calculated)	1.433 Mg/m^3	
Absorption coefficient	5.689 mm^{-1}	
F(000)	2000	
R_{wp}	0.0119	
R_p	0.0086	
R_F^2	0.0411	
CCDC reference number	869549	

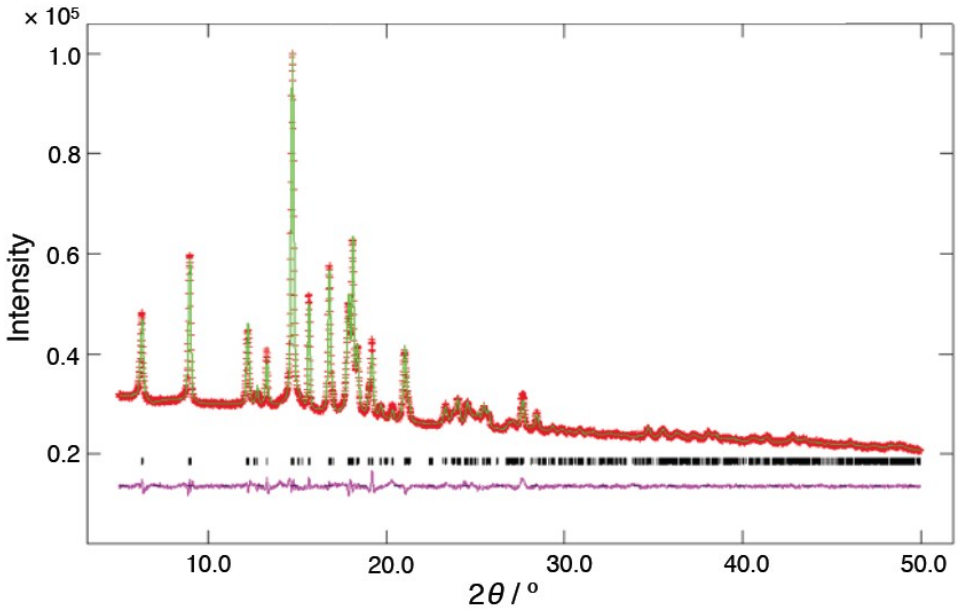


Fig. S16 Experimental (red), calculated (light green), and difference (pink) PXRD profiles from final Rietvelt refinement of *hetero*-**3**.

Single-crystal X-ray diffraction analysis and structure of 5

The single crystal X-ray diffraction data were recorded on a Rigaku R-AXIS RAPID (IP area detector system) at 173 K using Cu*K*α radiation. The structure was solved by direct methods using SHELXS-97 (G. M. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112.) and refined by full-matrix least squares using SHELXL-2016 (G. M. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3.). CCDC 1521416 contains the supplementary crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

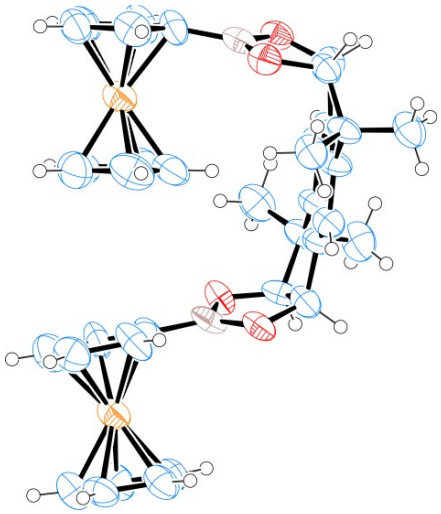


Fig. S17 ORTEP drawing (50% probability ellipsoids) of **5**.

Table S3. Crystal data and structure refinement for **5**.

Identification code	shelx
Empirical formula	$C_{72}\ H_{72}\ B_4\ Fe_4\ O_8$
Formula weight	1331.94
Temperature	173(2) K
Wavelength	1.54186 Å
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	*a* = 13.2454(5) Å
	b = 20.5430(8) Å
	c = 22.8531(9) Å
Volume	6218.3(4) $Å^3$
Z	4
Density (calculated)	1.423 Mg/m^3
Absorption coefficient	7.791 mm^{-3}
F(000)	2768
Crystal size	0.05 × 0.05 × 0.02 mm^3
Theta range for data collection	3.87 to 68.24 °.
Index ranges	–15<=h<=15, –24<=k<=23, –26<=l<=27
Reflections collected	54618
Independent reflections	5681 [R(int) = 0.1592]
Completeness to theta = 68.24 °	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8598 and 0.6967
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5681 / 0 / 398
Goodness-of-fit on F^2	1.172
Final R indices [I > 2sigma(I)]	R_1 = 0.1325, wR_2 = 0.3050
R indices (all data)	R_1 = 0.2120, wR_2 = 0.4094
Largest diff. peak and hole	0.612 and -1.159 e.$Å^{-3}$
CCDC reference number	1521416

Optimized structures and total energies of *homo*-**3** and *hetero*-**3** with DFT calculation

Optimizations of the geometries of *homo*-**3** and *hetero*-**3** were performed with DFT calculation at the B3LYP/6-31G* level (Gaussian 09).[S2] Both geometries were characterized to be minima with no imaginary frequencies by vibrational analysis. Total energies were corrected with zero-point energies.

[S2] Gaussian 09, Revision A.02, M. J. Frisch, et al., Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates of all optimized geometry and total energy of *homo*-**3**

E = –5240.840787 (au)

Standard Nuclear Orientation (Angstroms)

Atom	X	Y	Z
Fe	-2.1443290	3.0157250	-0.2788500
H	-4.1272500	3.5892680	-2.1795050
C	-3.6623270	3.9600630	-1.2751930
C	-2.5273230	4.8150740	-1.2109460
H	-1.9817230	5.2148440	-2.0560210
C	-2.2161090	5.0297290	0.1677700
H	-1.3915260	5.6182720	0.5492390
C	-3.1598850	4.3072640	0.9481230
H	-3.1786440	4.2482760	2.0286260
C	-4.0734780	3.6301910	0.0643270
H	-2.8329770	0.5781480	-1.5065730
C	-2.0549250	1.0718730	-0.9395650
C	-1.9623210	1.1146620	0.4859910
H	-0.7622420	1.9884720	-2.5177980
H	-2.6566030	0.6566370	1.1770800
C	-0.8256540	1.8941450	0.8292080
H	-0.4874870	2.1201780	1.8321170
C	-0.1870310	2.3405200	-0.3792490
C	-0.9709240	1.8232130	-1.4686950
B	-5.1145140	2.5709280	0.4717750
O	-5.3250580	2.1865970	1.7802540
O	-5.8992030	1.8746400	-0.4252570
C	-6.5408210	0.8126060	0.3078480

H	-7.5863990	0.7642910	-0.0134050
C	-6.3454630	1.1771640	1.8113670
H	-7.2350880	1.6118330	2.2817080
B	1.1468490	3.0990200	-0.4935910
O	1.7614070	3.3464360	-1.7025880
O	1.8973630	3.5176500	0.5865420
C	3.0306030	3.9716020	-1.4637960
H	2.9775630	5.0007980	-1.8370250
C	3.2017860	3.8681100	0.0837820
H	3.5134600	4.7993100	0.5679440
C	-5.8905190	-0.1201050	2.5449790
C	-5.3453210	-0.9656150	1.3955940
C	-5.7941600	-0.4942540	0.1530400
C	-7.1384370	-0.8148290	3.1414420
H	-7.9106270	-0.9837740	2.3815120
H	-7.5744910	-0.2068310	3.9434240
H	-6.8705350	-1.7904540	3.5615360
C	-4.8738940	0.1537430	3.6623140
H	-3.9749600	0.6403490	3.2774980
H	-4.5815760	-0.7814910	4.1537540
H	-5.3081090	0.8086870	4.4263700
H	-4.1230510	-2.4475880	2.4057070
C	-4.5219150	-2.0912300	1.4592000
H	-5.8373490	-0.7641930	-1.9887260
C	-5.4816870	-1.1517050	-1.0371270
C	-4.6684680	-2.2847180	-0.9721710
C	-4.1794180	-2.7273000	0.2652050
C	-3.2017850	-3.8681110	0.0837670
H	-3.5134580	-4.7993140	0.5679240
C	-4.2125890	-3.1893880	-2.1143860
C	-3.0306060	-3.9715910	-1.4638120
H	-2.9775670	-5.0007850	-1.8370480
C	-3.7909150	-2.4291170	-3.3801400
H	-3.4164280	-3.1234010	-4.1410330
H	-2.9991830	-1.7080910	-3.1650900

H	-4.6462410	-1.8951250	-3.8101420
C	-5.3421480	-4.1889880	-2.4583800
H	-5.0243870	-4.8759990	-3.2521920
H	-6.2340990	-3.6568320	-2.8067530
H	-5.6338580	-4.7857960	-1.5859730
O	-1.8973610	-3.5176550	0.5865270
O	-1.7614130	-3.3464220	-1.7026030
B	-1.1468500	-3.0990160	-0.4936060
Fe	2.1443270	-3.0157220	-0.2788670
H	0.7622410	-1.9884550	-2.5178080
C	0.9709220	-1.8232030	-1.4687040
C	2.0549240	-1.0718670	-0.9395700
H	2.8329760	-0.5781380	-1.5065760
C	1.9623200	-1.1146640	0.4859860
H	2.6566030	-0.6566440	1.1770770
C	0.8256530	-1.8941490	0.8291980
H	0.4874870	-2.1201880	1.8321060
C	0.1870290	-2.3405160	-0.3792610
H	1.9817040	-5.2148350	-2.0560440
C	2.5273120	-4.8150680	-1.2109710
C	2.2161060	-5.0297280	0.1677460
H	4.1272350	-3.5892620	-2.1795380
H	1.3915240	-5.6182700	0.5492170
C	3.1598870	-4.3072670	0.9480950
H	3.1786530	-4.2482830	2.0285980
C	4.0734770	-3.6301920	0.0642960
C	3.6623160	-3.9600590	-1.2752230
B	5.1145150	-2.5709320	0.4717430
O	5.8992000	-1.8746390	-0.4252890
O	5.3250660	-2.1866090	1.7802230
C	6.5408210	-0.8126100	0.3078190
H	7.5863980	-0.7642930	-0.0134390
C	6.3454710	-1.1771760	1.8113370
H	7.2350990	-1.6118480	2.2816700
C	4.2125820	3.1894020	-2.1143800

C	3.7909030	2.4291400	-3.3801380
H	2.9991710	1.7081130	-3.1650900
H	4.6462270	1.8951490	-3.8101460
H	3.4164150	3.1234290	-4.1410250
C	5.3421410	4.1890030	-2.4583710
H	5.6338540	4.7858050	-1.5859610
H	5.0243770	4.8760200	-3.2521780
H	6.2340900	3.6568490	-2.8067500
C	4.1794200	2.7272980	0.2652080
C	4.6684650	2.2847240	-0.9721730
C	5.8905310	0.1200880	2.5449590
C	4.8739110	-0.1537650	3.6622970
H	3.9749750	-0.6403700	3.2774820
H	4.5815960	0.7814660	4.1537430
H	5.3081290	-0.8087140	4.4263470
C	7.1384520	0.8148090	3.1414190
H	7.5745100	0.2068060	3.9433960
H	6.8705520	1.7904310	3.5615210
H	7.9106370	0.9837580	2.3814870
C	5.7941610	0.4942520	0.1530220
C	5.3453270	0.9656060	1.3955810
H	4.1230620	2.4475730	2.4057090
C	4.5219210	2.0912200	1.4591970
H	5.8373400	0.7642050	-1.9887430
C	5.4816830	1.1517110	-1.0371390

Cartesian coordinates of all optimized geometry and total energy of *hetero*-**3**

E = –5240.842153 (au)

Standard Nuclear Orientation (Angstroms)

Atom	X	Y	Z
Fe	2.2296290	-2.9270590	-1.2071160
H	4.4689010	-3.3936950	-2.8377800
C	3.9074410	-3.7831020	-1.9984500

C	2.8217130	-4.7012920	-2.0722400
H	2.4102850	-5.1316190	-2.9762370
C	2.3524630	-4.9327780	-0.7433810
H	1.5204590	-5.5663310	-0.4641220
C	3.1525960	-4.1622140	0.1468770
H	3.0358000	-4.1080530	1.2213340
C	4.1326000	-3.4386160	-0.6189050
H	2.2916870	-1.0596930	-3.3220030
C	1.7747190	-1.3175890	-2.4066040
C	2.1221030	-0.8741090	-1.0944950
H	0.1507380	-2.6877150	-3.1093940
H	2.9456280	-0.2189550	-0.8447800
C	1.2191210	-1.4757720	-0.1742770
H	1.2187580	-1.3388730	0.8989110
C	0.2862760	-2.2907980	-0.9056790
C	0.6505270	-2.1832670	-2.2922750
B	5.1170210	-2.3819600	-0.0811140
O	5.3241400	-2.1581540	1.2632790
O	5.8732020	-1.5544030	-0.8874140
C	6.4909570	-0.5786230	-0.0263020
H	7.5286630	-0.4501360	-0.3513670
C	6.3351470	-1.1485820	1.4151820
H	7.2388230	-1.6349620	1.8003900
B	-0.9043940	-3.0678710	-0.3137240
O	-1.9249980	-3.5968110	-1.0787270
O	-1.0939900	-3.2577400	1.0389320
C	-2.9740790	-3.9742610	-0.1679300
H	-3.3828260	-4.9350760	-0.4975730
C	-2.3048280	-4.0061170	1.2372930
H	-2.0289440	-5.0110410	1.5777260
C	5.8875450	0.0280680	2.3325090
C	5.3082040	1.0171300	1.3248050
C	5.7035430	0.7134290	0.0138370
C	7.1404760	0.6425240	3.0001560
H	7.8972580	0.9237280	2.2581880

H	7.5955350	-0.0679200	3.7009500
H	6.8738020	1.5466470	3.5582130
C	4.8880440	-0.4121740	3.4120230
H	3.9826190	-0.8317740	2.9680400
H	4.6058000	0.4379470	4.0439170
H	5.3322460	-1.1757840	4.0607340
H	4.1297450	2.3467430	2.5714890
C	4.4831740	2.1156100	1.5699110
H	5.5994790	1.2217910	-2.0821380
C	5.3035500	1.4939120	-1.0720600
C	4.4684150	2.5858830	-0.8279370
C	4.0659710	2.8819930	0.4823040
C	3.0673910	4.0192330	0.4982990
H	3.4286920	4.9191600	1.0064540
C	3.8732400	3.5701030	-1.8328250
C	2.7233170	4.2206370	-1.0069650
H	2.5634380	5.2665210	-1.2937220
C	3.3696300	2.9061580	-3.1228200
H	2.8834430	3.6436760	-3.7717540
H	2.6457860	2.1172630	-2.9066120
H	4.2061440	2.4719340	-3.6828990
C	4.9167240	4.6587090	-2.1775080
H	4.4947100	5.3967600	-2.8705830
H	5.7958820	4.2107180	-2.6533290
H	5.2611290	5.1889490	-1.2816100
O	1.8330080	3.6162880	1.1194410
O	1.4743910	3.5240410	-1.1508770
B	0.9962280	3.2019190	0.1017370
Fe	-2.2571070	2.9584120	0.5306720
H	-0.9605500	1.8663020	-1.7384540
C	-1.0992200	1.7579330	-0.6708170
C	-2.1051490	0.9829800	-0.0337840
H	-2.8807670	0.4123780	-0.5273340
C	-1.9352230	1.1158500	1.3793250
H	-2.5685480	0.6725510	2.1355760

C	-0.8180960	1.9657870	1.6066150
H	-0.4341570	2.2696450	2.5720210
C	-0.2793500	2.3745460	0.3374540
H	-1.7524480	5.5178780	-0.5719280
C	-2.4894100	4.9282380	-0.0419740
C	-2.6034280	4.8048580	1.3775980
H	-3.6501640	3.9737850	-1.6973360
H	-1.9726000	5.2899250	2.1113180
C	-3.6741740	3.9093170	1.6536330
H	-3.9981860	3.5884960	2.6353120
C	-4.2432650	3.4659330	0.4079420
C	-3.4914990	4.1125900	-0.6358160
B	-5.2809210	2.3428790	0.2237990
O	-5.7779320	1.9627410	-1.0052840
O	-5.7836950	1.5871000	1.2646640
C	-6.7273740	0.9012510	-0.8135310
H	-7.7258190	1.3016890	-1.0239500
C	-6.5106970	0.4924890	0.6741560
H	-7.4351140	0.3537570	1.2442830
C	-3.2856210	-3.3161150	2.2307130
C	-4.1670280	-4.4007760	2.8943230
H	-4.9451580	-3.9382830	3.5113240
H	-3.5635680	-5.0507040	3.5397260
H	-4.6680450	-5.0292950	2.1484550
C	-2.5549850	-2.5088620	3.3132550
H	-1.9134540	-3.1632570	3.9147340
H	-3.2749370	-2.0364130	3.9918520
H	-1.9259400	-1.7328010	2.8720910
C	-6.4208000	-0.3521460	-1.6859440
C	-4.0147180	-2.8823300	-0.0389800
C	-4.1401900	-2.4651920	1.2940880
C	-7.7461130	-1.1014940	-1.9612460
H	-8.2819140	-1.3300040	-1.0322980
H	-7.5510250	-2.0508820	-2.4718080
H	-8.4067790	-0.5018760	-2.5991210

C	-5.7416720	0.0040880	-3.0159890
H	-4.7949230	0.5236520	-2.8526670
H	-6.3859100	0.6571620	-3.6157750
H	-5.5472380	-0.9011640	-3.6027120
C	-5.6613090	-0.7574690	0.5800100
C	-5.5492440	-1.1869300	-0.7507140
H	-5.0640040	-1.0309760	2.6364510
C	-4.9755860	-1.3938290	1.6152970
H	-4.5854750	-2.5881290	-2.0998010
C	-4.7193640	-2.2628330	-1.0712330
