shortest Cu···Cu distances in $[Cu_4(mhp)_4]$ also suggests a weak bond at most, with significant accommodation to crystal packing forces.

We note that in $[Cu_4(mhp)_4]$ the mhp ligand does not produce a notably short metal–metal separation. This is in contrast to the $[M_2(mhp)_4]$ complexes, in which the separations are among the very shortest observed for each metal.[2a,3–6] Clearly, a single mhp bridge is much less effective in this respect than a set of four.

Spectra. The ^1H NMR spectrum of $[Cu_4(mhp)_4]$ is consistent with equivalence of all the mhp groups, for a solution in $CDCl_3$ at room temperature. A single peak is observed at a τ value of 7.43; this is assigned[24] to the four equivalent methyl groups, and the peak area is scaled to be equal to 12 atoms. There is an overlapping pair of doublets, centered at τ 3.91, with a total area corresponding to eight hydrogen atoms, and this is attributed to the hydrogen atoms attached to C-3 and C-5 atoms split by coupling to the hydrogen attached to C-4. The latter atom is considered to give rise to the doublet of doublets centered at τ 3.02, with a total area corresponding to four hydrogen atoms.

The mass spectrum of $[Cu_4(mhp)_4]$ contains as its highest intensity feature a peak at an m/e value of 342; this is the lowest m/e feature in a set of adjacent peaks that extend to 347. The m/e values of these peaks and their relative intensities correspond very closely to those expected for the $Cu_2(mhp)_2^+$ ion. A reasonably intense set of peaks is observed between m/e values of 234 and 239, with an intensity profile expected for $Cu_2(mhp)^+$; a less intense set of four peaks is observed between m/e 171 and 174, and these values, together with their intensity profile, are consistent with the formation of $Cu(mhp)^+$. Peaks are also observed at higher (>300) m/e values, consistent with the formation of $Cu_4(mhp)_3^+$, $Cu_4(mhp)_2^+$, and $Cu_4(mhp)^+$ ions; they have, however, very low intensity, compared with the peaks corresponding to $Cu_2(mhp)_2^+$. Therefore, in one sense, the mass spectrum of $[Cu_4(mhp)_4]$ differs from those of $[M_2(mhp)_4]$ (M = Cr, Mo, W;[2a,24] Ru, Rh[24]), since all of the latter molecules show clear evidence for the production of the corresponding molecular ion. In another sense, however, $[Cu_4(mhp)_4]$ resembles these other mhp complexes in that its mass spectrum is dominated by ions that contain two metal atoms. As discussed for $[Pd_2(mhp)_4]$,[6] the fragmentation of $[Cu_4(mhp)_4]$ is consistent with a very weak net bonding attraction between the metal atoms (vide supra); a rearrangement of the bridging mhp groups is presumed to occur upon the dissociation of the Cu_4 tetramer to the Cu_2 dimer, with the latter involving two mhp groups bridging the two metal atoms.

Acknowledgment. We thank the Science Research Council (M.B., C.D.G., and I.H.H.) and the Verband der Chemischen Industrie (W.C.) for financial support.

Registry No. $Cu_4(mhp)_4$, 80301-55-9.

Supplementary Material Available: Tables of observed and calculated structure factors, anisotropic thermal parameters, and hydrogen atom parameters (15 pages). Ordering information is given on any current masthead page.

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[24] Garner, C. D.; Berry, M.; Al-Samman, M. H., unpublished results.

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X-ray Crystal Structure of a Tetrabridged Ferrocenophane Trimer: 6,9,12-Trioxo[3.3.3](1,1′)[4](2,2′)[4](3,3′)[4](4,4′)[4](5,5′)ferrocenophane[1,2]

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The structure of the tetrabridged ferrocenophane trimer **3**, synthesized by treatment of $[4_4]$ferrocenophanepropionic acid (**2**) with polyphosphate ester, has been determined by the X-ray crystallographic method. The compound is the first intermolecular [3.3.3](1,1′)ferrocenophane composed of three cage-type ferrocene moieties. It was crystallized from $CDCl_3$ as $(C_{29}H_{36}OFe)_3 \cdot 2CDCl_3$ in space group $P2_1nb$ with four molecules per unit cell of dimensions $a = 23.30$ (2) Å, $b = 21.69$ (2) Å, $c = 14.94$ (1) Å, $D_m = 1.399$ g cm^{-3}, $D_x = 1.416$ g cm^{-3}, $R = 0.083$, and $R_w = 0.0091$. The molecule of **3** is characterized by a macrocyclic structure with a pseudo-D_3 symmetry having a screw conformation of the tetramethylene bridges. For the methylene carbon atoms, no unusual anisotropy of the thermal vibration was found even though it was commonly observed in bridged ferrocene molecules previously determined.

Introduction

Previously, we reported synthesis of tetrabridged ferrocenophanes and their molecular structures by X-ray crystallographic analysis.[6,7] As a step to synthesize pentabridged ferrocenophane ("superferrocenophane"[8]), a novel cage compound containing an iron atom in the center of the molecule, $[4_4]$ferrocenophanepropionic acid (**2**) was synthesized via several steps from tetrabridged ferrocenophane **1**. However, an attempt at the formation of the last bridge by cyclization of propionic acid (**2**) resulted in the production of a ferrocenophane trimer (**3**) as the major product besides certain other intramolecular cyclization product.[10] The interesting macrocyclic trimer **3** is the first example of [3.3.3](1,1′)-ferrocenophane consisting of both inter- and intramolecular

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(1) Organometallic Compounds. 33. For part 32, see ref 4.

(2) The nomenclature of ferrocenophanes in the present paper is according to that presented by Vögtle and Neumann.[5] The numbering of the atoms is shown in Figure 1.

(3) (a) Science University of Tokyo. (b) University of Tokyo.

(4) Hisatome, M.; Tachikawa, O.; Sasho, M.; Yamakawa, K. *J. Organomet. Chem.* **1981**, *217*, C17.

(5) Vögtle, F.; Neumann, P. *Tetrahedron* **1970**, *26*, 5847.

(6) Hisatome, M.; Kawajiri, Y.; Yamakawa, K.; Iitaka, Y. *Tetrahedron Lett.* **1979**, 1777.

(7) (a) Kawajiri, Y.; Hisatome, M.; Yamakawa, K., paper presented at the 12th Symposium on Structural Organic Chemistry, Matsumoto, Japan, Sept 29–30, 1979. The authors reported on synthesis and X-ray crystallographic analysis of [4](1,1′)[4](2,2′)[4](3,3′)[4](4,4′)-ferrocenophane at the symposium. (b) Iitaka, K.; Ohnishi, H., manuscript on the above X-ray crystal structure in preparation.

(8) The pentabridged ferrocenophane may be named "superferrocenophane" as a ferrocene analogue of Boekelheide's "superphane".[9]

(9) (a) Sekine, Y.; Brown, M.; Boekelheide, V. *J. Am. Chem. Soc.* **1979**, *101*, 3126. (b) Sekine, Y.; Boekelheide, V. *Ibid.* **1981**, *103*, 1777.

(10) The synthesis of propionic acid (**2**) will be published elsewhere together with the result on the structure of the intramolecular cyclization product, whose X-ray crystallographic analysis is in progress.

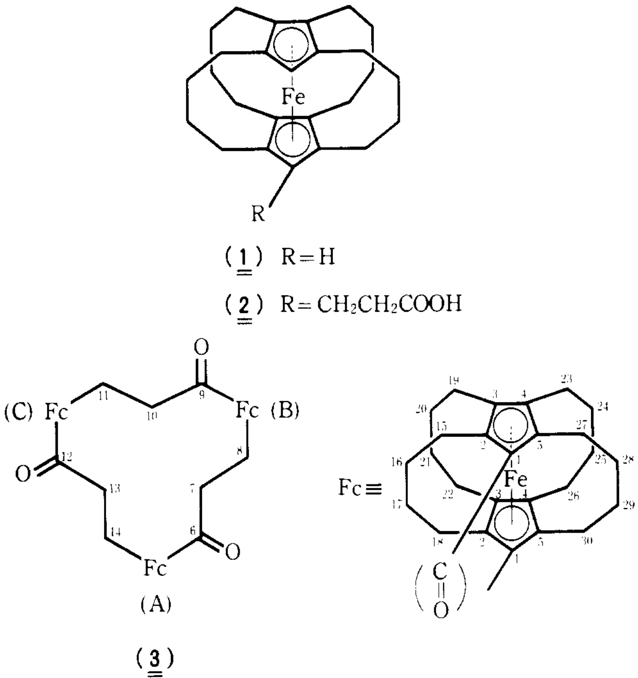

Figure 1. Chemical structure of three ferrocenophanes and the numbering of atoms in trimer **3**. Three tetrabridged ferrocene moieties of **3** are named A, B, and C as illustrated.

phane structure. There have been reports on intermolecular [1.1.1]- and [2.2.2](1,1′)ferrocenophanes[11,12] formed by ferrocene synthesis of cyclopentadienyl (Cp) derivatives, as cyclic ferrocene trimers. We wish to report the characterization and structure determination of the trimer **3** by X-ray crystallographic study.

Experimental Section

Material. The trimer **3** was isolated from a band of preparative TLC (silica gel) of the cyclization products of **2**[10] with polyphosphate ester (PPE) in dichloromethane at 80 °C. The compound **3** (orange yellow amorphous solid), which showed a C=O stretching band at 1660 cm^{-1} in the IR spectrum, gave the $[M + 1]^+$ ion peak corresponding to the trimer $[(C_{29}H_{36}OFe)_3$: mol wt 1368] at *m/z* 1369 in the FD mass spectrum. Neither the peak of a Cp ring proton nor an unsubstituted Cp ring carbon was observed in the ^{1}H and ^{13}C NMR spectra. Various attempts at the crystallization of the trimer **3** from common solvents were unsuccessful. The orange rectangular parallelepiped crystals (mp 451 °C dec[13]) were grown from $CDCl_3$ solution prepared for NMR measurement and were used for the present X-ray crystallographic study.

X-ray Data Collection. A rodlike crystal of dimensions 0.3 × 0.15 × 0.1 mm^3 of **3** was used for data collection at room temperature. The lattice parameters and intensity data were measured on a Philips PW-1100 automatic four-circle diffractometer by means of the $\theta-2\theta$ scan method with a scan speed of 6° 2θ min^{-1} by using graphite-monochromated Co Kα radiation. Crystal data are given in Table I. The intensities of 3491 independent reflections $[I_o > 2\sigma(I_o)]$ were obtained within θ_{max} of 78°, corresponding to about 66% of the theoretically possible reflections within the same angular range. Lorentz and polarization corrections as well as absorption correction by crystal shape[14] were applied for the observed intensity data.

Structure Determination. A careful observation of the intensity data revealed a systematic extinction of *P*2$_1$*nb*. However, the intensities of $l = 2n + 1$ reflections in $(0kl)$ were systematically very weak (confirmed by taking a precession photograph) compared with those of $l = 2n$. The space group was then considered to be approximately *Pcnb* in which the molecule must have its own symmetry 2 or $\bar{1}$ coinciding with the symmetry element of the space group. Disposition of heavy atoms (Fe and Cl) was determined by the Patterson map interpretation. The location of lighter atoms was determined by successive calculations of difference electron density map and block-diagonal-matrix least-squares procedures. The refinement was carried out by the same least-squares procedure, allowing for the anisotropic thermal vibrations for all atoms and fixing the *x* coordinate of the Fe(A) atom. Chirality of crystal was determined by comparison of *R* including an anomalous dispersion effect (Fe: $f' = -3.507, f'' = 0.656$. Cl: $f' = 0.357, f'' = 0.935$). No attempt was made to locate hydrogen atoms. The final *R* and R_w $[\sum w(F_o^2 - |F_c|^2)/\sum wF_o^2]$ values were reduced to 0.083 and 0.0091, respectively. No peak higher than 0.5 e/Å^3 appeared on the final difference map. The atomic positional parameters are given together with their standard deviations in Table II. The molecular structure is illustrated in Figures 2 and 3 by ORTEP drawings with 20% probability thermal ellipsoids.

Table I. Crystal Data for $C_{87}H_{108}O_3Fe_3 \cdot 2CDCl_3$ (3)

mol wt: 1608.1
cryst system: orthorhombic
space group: $P2_1nb$
$a = 23.30$ (2) Å
$b = 21.69$ (2) Å
$c = 14.94$ (1) Å
$Z = 4$

$V = 7550$ (18) Å^3
$D_x = 1.416$ g cm^{-3}
$D_m = 1.399$ g cm^{-3}
$\lambda = 1.7902$ Å (Co Kα)
temp: 23 (1) °C
μ(Co Kα) = 46.2 cm^{-1}
$\exp(-d_{min}\mu) = 0.630$
$\exp(-d_{max}\mu) = 0.250$

Results and Discussion

The present analysis revealed a unique structure produced by the intermolecular condensation reaction among three molecules of tetrabridged ferrocenophane propionic acid (**2**). The trimer has a pseudo-C_3 axis (Figure 2 is drawn nearly along the C_3) and three additional pseudo-C_2 axes perpendicular to the C_3 axis (Figure 3 shows the molecule viewed nearly along one of the C_2 axis). Thus the molecule has pseudo-D_3 symmetry even though the carbonyl groups at the methylene bridges connecting two ferrocene moieties disturb the exact C_2 symmetry.

The crystal contains two stoichiometric $CDCl_3$ for one molecule of the trimer, and the $CDCl_3$ molecules interact with the trimer by filling the central cavity of the macrocyclic ring as shown in Figures 2 and 3. The carbonyl groups on the intermolecular methylene chains extend to the cavity and possibly form hydrogen bonds [O(6)···D–C(Cl) and O(12)···D–C(Cl′)], with the O···C distances of 3.13 (3) and 3.13 (3) Å, respectively. It seems that the $CDCl_3$ molecules play an important role in crystallization of the trimer **3** because any attempt at the crystallization of **3** from other common solvents was unsuccessful.

Figure 4 shows the averaged bond lengths and averaged bond angles. Almost all of the bond lengths and angles are in normal ranges.[6,7,15-18]

The conformations of the methylene chains in the three ferrocene moieties, A, B, and C, are compared in Figure 5, where A and B are the moieties related by a pseudo-C_2 axis. It is noted that the rotations along all the methylene C–C bonds are plus or minus gauche and that there are two types of the conformations for the methylene bridges: dextro screw and levo screw. All Cp rings show a good planarity and the average value of the atomic deviations from its own least-squares plane is about 0.01 Å (root mean square), but all

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(11) (a) Katz, T. G.; Acton, N.; Martin, G. *J. Am. Chem. Soc.* **1969**, *91*, 2804. (b) Lippard, S. J.; Martin, G. *Ibid.* **1970**, *92*, 7291.

(12) Lentzner, H. L.; Watts, W. E. *Tetrahedron* **1971**, *27*, 4343.

(13) The datum was obtained on a Perkin-Elmer DSC-2C calorimeter.

(14) Wuensch, B. J.; Prewitt, C. T. *Z. Kristallogr.* **1965**, *122*, 25.

(15) (a) Hillman, M.; Fujita, E. *J. Organomet. Chem.* **1978**, *155*, 87. (b) Hillman, M.; Fujita, E. *Ibid.* **1978**, *155*, 99. (c) Spaulding, L. D.; Hillman, M. *Ibid.* **1978**, *155*, 109. (d) Hillman, M.; Gordon, B.; Dudek, N.; Fajor, R.; Fujita, E.; Gaffney, J.; Jones, P.; Weiss, A. J.; Takagi, S. *Ibid.* **1980**, *194*, 229.

(16) Cameron, T. S.; Cordes, R. E. *Acta Crystallogr., Sect. B* **1979**, *B35*, 748.

(17) Fujita, E.; Hillman, M., private communication. The X-ray crystallographic analysis of [4](1,1′)[4](2,2′)[4](4,4′)ferrocenophane has been completed by them.

(18) Willi, C.; Reis, A. H., Jr.; Gebert, E.; Miller, J. S. *Inorg. Chem.* **1981**, *20*, 313.

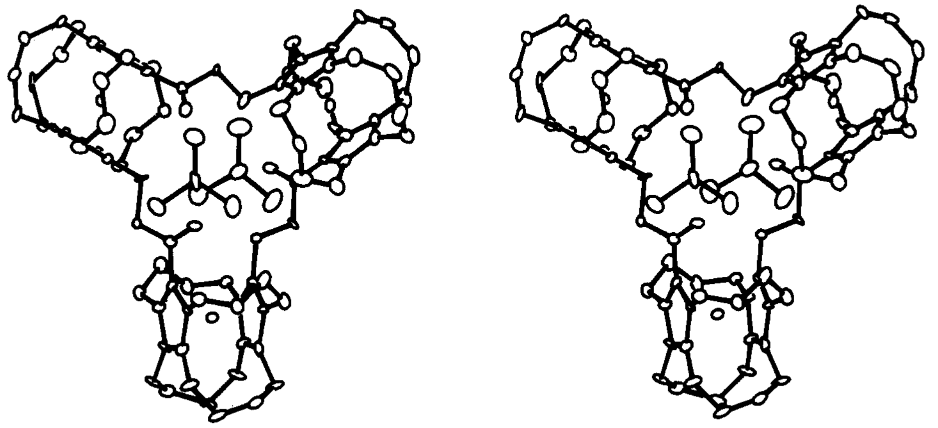


Figure 2. Stereoscopic drawing of trimer **3** viewed perpendicular to the plane formed by the three iron atoms. The pseudo-C_3 axis runs through the center of the molecule. The atoms are drawn with 20% probability ellipsoids.

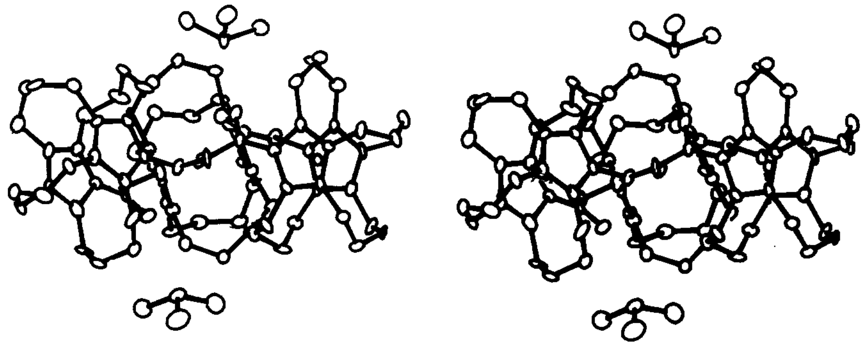
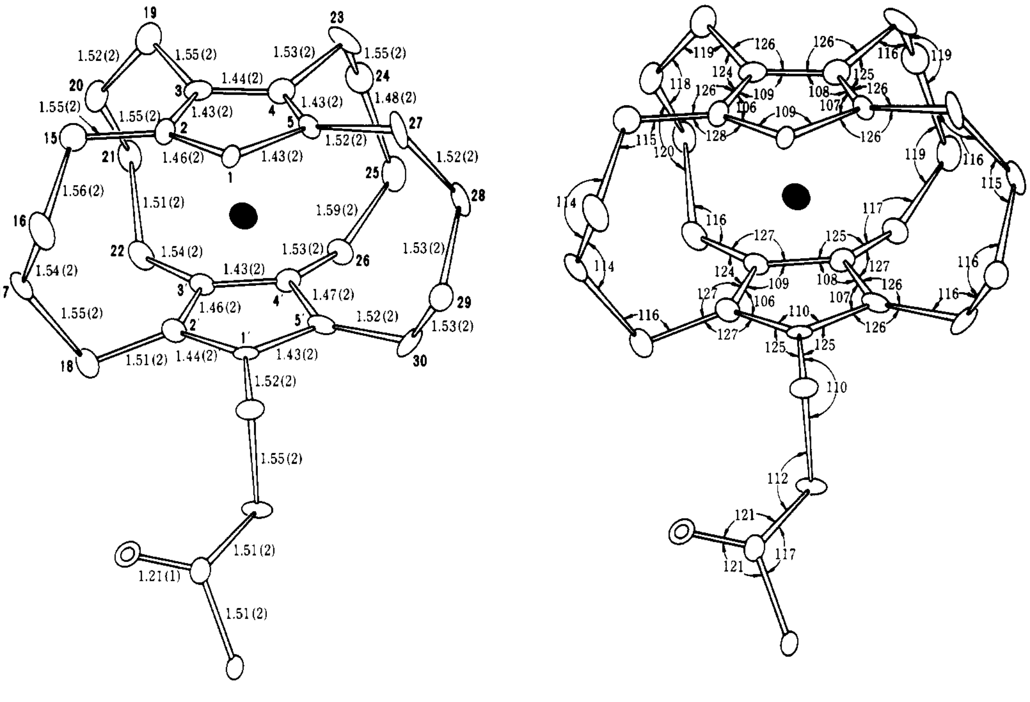


Figure 3. Stereoscopic drawing of trimer **3**. The plane formed by the three iron atoms are perpendicular to the paper. The pseudo-C_2 axis runs perpendicular to the paper through the center of the figure.



(a) (b)

Figure 4. Bond lengths and angles averaged for A, B, and C moieties. Single, double, and black circles in the figures represent carbon, oxygen, and iron atoms, respectively. (a) The averaged bond lengths with their estimated standard deviations in Å. (b) The averaged bond angles in degrees. Esd's are about 1.5° with the maximum value of 2.2°.

carbon atoms linked directly to the Cp ring deviate about 0.15 Å (root mean square) from this plane in the opposite direction to the iron atom. Two Cp rings in each ferrocene moiety are almost stacked parallel to each other, and the dihedral angles between the two Cp rings are 2.4, 3.2, and 2.9° for the moieties A, B, and C, respectively, as observed in the other symmetric multibridged ferrocenophanes.[7,15a,17]

The remarkable structural characteristics of this trimer **3** are as follows: (i) the absence of disorder in the methylene carbon chains which has been commonly observed in the tri-

Table II. Atomic Coordinates ($\times 10^4$) with Estimated Standard Deviations in Parentheses

atom	*x*	*y*	*z*
Fe(A)	−106 (0)	2410 (2)	−3783 (2)
C(A1)	−807 (8)	2599 (8)	−3027 (11)
C(A2)	−667 (8)	3123 (8)	−3547 (11)
C(A3)	−689 (8)	2925 (8)	−4459 (11)
C(A4)	−858 (8)	2270 (8)	−4487 (12)
C(A5)	−906 (7)	2056 (8)	−3583 (10)
C(A1′)	575 (8)	2186 (9)	−2966 (11)
C(A2′)	731 (8)	2727 (8)	−3444 (10)
C(A3′)	693 (8)	2581 (8)	−4403 (11)
C(A4′)	515 (7)	1937 (7)	−4506 (12)
C(A5′)	439 (7)	1688 (8)	−3578 (10)
C(A15)	−555 (9)	3791 (8)	−3245 (12)
C(A16)	−36 (9)	3879 (9)	−2622 (14)
C(A17)	552 (8)	3906 (8)	−3133 (14)
C(A18)	915 (8)	3309 (9)	−3026 (12)
C(A19)	−630 (10)	3338 (9)	−5282 (12)
C(A20)	−93 (10)	3644 (8)	−5517 (12)
C(A21)	425 (9)	3199 (9)	−5806 (12)
C(A22)	896 (9)	3000 (8)	−5151 (11)
C(A23)	−1014 (9)	1873 (9)	−5298 (11)
C(A24)	−511 (9)	1763 (10)	−6012 (12)
C(A25)	−68 (9)	1304 (9)	−5714 (12)
C(A26)	562 (11)	1576 (10)	−5356 (12)
C(A27)	−1158 (9)	1446 (8)	−3301 (12)
C(A28)	−775 (9)	894 (8)	−3458 (13)
C(A29)	−232 (9)	875 (9)	−2869 (15)
C(A30)	318 (9)	1016 (8)	−3380 (14)
C(6)	−892 (8)	2540 (8)	−2004 (11)
C(7)	−1221 (7)	3022 (7)	−1580 (10)
C(8)	−1184 (9)	2943 (8)	−528 (10)
O(6)	−738 (6)	2074 (6)	−1627 (7)
Fe(B)	−1447 (1)	3711 (1)	1280 (2)
C(B1)	−956 (8)	3089 (8)	1954 (10)
C(B2)	−741 (7)	3710 (8)	2131 (11)
C(B3)	−1200 (7)	4055 (9)	2520 (11)
C(B4)	−1672 (7)	3650 (7)	2638 (11)
C(B5)	−1536 (7)	3062 (8)	2273 (10)
C(B1′)	−1477 (8)	3487 (7)	−67 (10)
C(B2′)	−1206 (7)	4087 (7)	86 (10)
C(B3′)	−1627 (8)	4461 (8)	528 (11)
C(B4′)	−2131 (7)	4103 (9)	662 (10)
C(B5′)	−2027 (7)	3471 (8)	339 (10)
C(B15)	−123 (8)	3966 (10)	1970 (13)
C(B16)	87 (8)	3932 (10)	985 (13)
C(B17)	−156 (9)	4458 (9)	420 (13)
C(B18)	−603 (9)	4266 (9)	−288 (11)
C(B19)	−1158 (9)	4721 (8)	2923 (13)
C(B20)	−1081 (9)	5259 (8)	2280 (14)
C(B21)	−1579 (8)	5391 (7)	1658 (14)
C(B22)	−1514 (10)	5176 (8)	671 (12)
C(B23)	−2231 (9)	3814 (9)	3133 (12)
C(B24)	−2611 (8)	4318 (10)	2732 (13)
C(B25)	−2932 (9)	4166 (10)	1920 (13)
C(B26)	−2689 (9)	4389 (10)	987 (15)
C(B27)	−1893 (9)	2460 (8)	2333 (13)
C(B28)	−2457 (9)	2436 (9)	1801 (15)
C(B29)	−2360 (9)	2410 (11)	811 (18)
C(B30)	−2473 (9)	2990 (10)	255 (13)
C(9)	−622 (8)	2568 (8)	1556 (12)
C(10)	−11 (9)	2430 (11)	1972 (10)
C(11)	416 (9)	2220 (8)	1272 (14)
O(9)	−848 (6)	2188 (6)	1094 (9)
Fe(C)	1439 (1)	1199 (1)	1146 (2)
C(C1)	1578 (7)	1498 (8)	−130 (10)
C(C2)	2098 (9)	1617 (11)	424 (13)
C(C3)	2249 (8)	1027 (9)	768 (13)
C(C4)	1884 (9)	562 (9)	415 (14)
C(C5)	1478 (9)	858 (8)	−150 (12)
C(C1′)	766 (7)	1692 (8)	1655 (12)
C(C2′)	1272 (7)	1784 (9)	2199 (11)
C(C3′)	1438 (8)	1139 (8)	2486 (10)
C(C4′)	1043 (8)	719 (7)	2109 (13)
C(C5′)	631 (7)	1059 (8)	1607 (12)
C(C15)	2418 (8)	2238 (10)	523 (13)
C(C16)	2394 (9)	2550 (10)	1483 (17)
C(C17)	1800 (9)	2770 (9)	1793 (14)
C(C18)	1549 (11)	2360 (9)	2548 (14)
C(C19)	2825 (7)	945 (10)	1277 (16)
C(C20)	2789 (9)	685 (9)	2259 (17)
C(C21)	2484 (9)	1057 (11)	3002 (12)
C(C22)	1879 (8)	970 (9)	3177 (12)
C(C23)	2016 (10)	−117 (10)	474 (14)
C(C24)	1573 (10)	−485 (10)	990 (18)
C(C25)	1466 (11)	−424 (8)	1957 (14)
C(C26)	1000 (9)	7 (10)	2301 (15)
C(C27)	1039 (10)	515 (10)	−708 (16)
C(C28)	425 (10)	677 (13)	−504 (16)
C(C29)	145 (8)	386 (9)	331 (14)
C(C30)	74 (8)	828 (11)	1135 (14)
C(12)	1305 (6)	1996 (7)	−653 (10)
C(13)	1194 (8)	1884 (8)	−1637 (11)
C(14)	584 (8)	2099 (9)	−1956 (11)
O(12)	1214 (6)	2512 (5)	−347 (7)
C(Cl)	−1474 (10)	1137 (10)	−513 (17)
Cl(1)	−2084 (3)	1403 (3)	−1109 (4)
Cl(2)	−1713 (4)	860 (3)	533 (4)
Cl(3)	−1201 (3)	484 (3)	−1100 (5)
C(Cl′)	1610 (11)	3872 (9)	−489 (14)
Cl(1′)	2163 (3)	3648 (4)	−1181 (6)
Cl(2′)	1879 (5)	4183 (4)	535 (5)
Cl(3′)	1185 (4)	4406 (4)	−1013 (6)

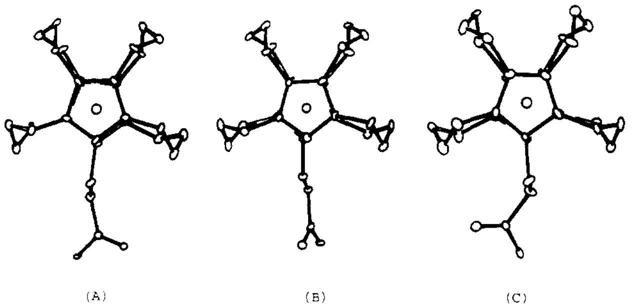


Figure 5. Comparison of the three fragment conformations of trimer **3**. Moiety A includes atoms Fe(A), C(A1)–C(A30), C(12)–C(14), and O(12). Moiety B includes atoms Fe(B), C(B1)–C(B30), C(6)–C(8), and O(6). Moiety C includes atoms Fe(C), C(C1)–C(C30), C(9)–C(11), and O(9).

and tetramethylene bridges of ferrocenophanes[6,7,18] and (ii) the novel screw conformation of the tetramethylene bridges. These two characteristics i and ii seem to be related to one another and can be explained by the number of methylene bridges and the number of methylene carbons in a bridge. In fact, structural investigations on some bridged ferrocenophanes by the X-ray diffraction method[6,7,15] have revealed the two common structural features: (i) the mean ring–ring distance is 3.3 Å and (ii) the carbon atoms linked directly to the Cp ring deviate generally "inside" from the ring plane to the iron atom in the case of trimethylene bridge and deviate "outside" in the case of tetramethylene bridges. These results suggest that (i) the coordination force of the Cp ring on iron is very strong and (ii) the trimethylene bridge is too short in length, while tetramethylene one is too long to connect fitly the two Cp rings. In case of the trimer **3**, the molecular structure is much more compact than that of the other ferrocenophanes previously synthesized[6,7] because each monomer unit involves four tetramethylene bridges and one α-oxomethylene chain that connects the monomer with the other. It is therefore most probable that the methylene chains are constrained to take a specific structure to accommodate the relatively small room. This is the reason why the crystals of the trimer **3** do not show a disordered structure.

Registry No. **3**, 80584-49-2.

Supplementary Material Available: Tables of observed and calculated structure factors, anisotropic temperature factors, bond lengths, bond angles, and least-squares planes through Cp rings (23 pages). Ordering information is given on any current masthead page.