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The Crystal Structure of 1,1'-dimethylferricenium Tri-iodide

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The crystal structure of 1,1'–dimethylferricenium tri-iodide has been determined from three-dimensional X-ray data collected by counter methods, and refined by least-squares techniques to a final conventional R factor, based on F, of 3.5%, for 1278 independent reflections. The material crystallizes in a triclinic cell, space group $P\bar{1}$, with dimensions $a=14.70(1)$, $b=7.440(6)$, $c=7.97(1)$ Å, $\alpha=70.50(3)°$, $\beta=81.49(3)°$ $\gamma=97.33(4)°$, $Z=2$. Although the two independent tri-iodide anions in the structure lie at crystallographic centres, refinement of a structural model with a 50:50 disorder of asymmetric anions about the centres of symmetry gave a significantly better fit to the data than refinement of a model based on centrosymmetric anions. The I–I distances in the asymmetric anions are 2.85(2) 2.97(2) Å for one, and 2.86(3) and 3.00(3) Å for the other. The cyclopentadienyl rings in the cation are almost exactly eclipsed with the methyl groups adjacent. The rings are inclined at 6.6° to each other. Mean distances are Fe-ring (perpendicular) = 1.695(1), Fe–C(ring) = 2.073(5), C–C(ring) = 1.401(5), C–CH_3 = 1.49(1) Å.

Introduction

Although ferrocene and its derivatives have been the subject of numerous structural studies in recent years[1], surprisingly little information is avaible on compounds containing the ferricenium cation. From ESR and NMR measurements on 1,1'– dimethylferricenium tri-iodide, Prins[2] of this Laboratory estimated a value of 1.93 Å for the Fe–ring distance, and pointed out that such a distance is reasonable in view of the fact that the ferricenium cation is less stable than ferrocene, in which the Fe-ring distance is 1.66 Å[3].

Bernstein and Herbstein[4] recently carried out a crystal structure analysis on ferricenium tri–iodide. Unfortunately, crystal disorder prevented them from gaining detailed information on the cation from this study, but they did find that the Fe–ring distance was of the order of 1.65 Å, the same as in ferrocene.

In view of the large discrepancy between these results, we have determined the crystal structure of 1,1' –dimethylferricenium tri–iodide in which no disorder problem was found.

Experimental Section

Crystals of 1.1'–dimethylferricenium tri–iodide suitable for X–ray structural work were supplied by R. Prins. Preliminary precession photographs showed that they belonged to the triclinic system. The cell dimensions were determined from a least–squares refinement of the θ values of several reflections measured on a Nonius three circle diffractometer using Mo (Kα) radiation (λ = 0.7107 Å). The results were: a = 14.70(1), b = 7.440(6), c = 7.97(1) Å, α = 70.50(3)°, β = 81.49(3)°, γ = 97.33(4)°. The standard deviations quoted here are five times the results obtained from the refinement program.

An irregularly shaped crystal with a maximum dimension of 0.25 mm. was aligned along the (401) axis on a Nonius three circle diffractometer, and the intensities of a complete set of independent reflections with $\theta \leqslant 20°$ were measured using a θ–2θ scan with Zr–filtered Mo K radiation. The background was counted for one half the scan time at each end of the scan. A total of 1278 reflections were found to have intensities significantly above background. As a check on the stability of both the crystal and the eletronic equipment, the intensity of a control reflection was measured every 100 reflections. No variation in the intensity of this reflection was detected.

The data were corrected for background, and Lorentz and polarization factors were applied. The standard deviation of an intensity I, σ(I), was then estimated from the following expression:

$$\sigma^2(I) = (CINT + BH + BL + (pI)^2),$$

where CINT is the total integrated peak count, BH and BL are the background counts, and I = CINT–(BH + BL). The factor p may be regarded as an ignorance factor[5], and has been included to prevent unreasonably high weight being given to the strong reflections. For this case p was taken as 0.35.

An empirical absorption correction was made using the method of Furnas[6]. The intensity of the 401 reflection was plotted as a function of φ, and the factors required to make this intensity independent of φ were applied to the rest of the data as an absorption correction. These factors ranged from 1.0 to 0.6.

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(6) T.C. Furnas, « Single Crystal Orienter Instruction Manual », General Electric Co., U.S.A., 1966.

Solution and Refinement of the Structure

In the least–squares refinements, the function minimized was $\Sigma(|Fo|-|Fc|)^2$ where $|Fo|$ and $|Fc|$ are the observed and calculated structure amplitudes, respectively, and $w=1/\sigma^2(Fo)$. The standard deviation of Fo, $\sigma(Fo)$, was taken as $\sigma(Fo^2)/(2Fo)$. The residuals R_1 and R_2 defined as $R_1=\Sigma(||Fo|-|Fc||)/\Sigma|Fo|$ and $R_2=[\Sigma w(|Fo|-|Fc|)^2/\Sigma w|Fo|^2]^{1/2}$.

In the structure factor calculations allowance for the anomalous scattering of iodine and iron was made using the method of Ibers and Hamilton.[7] All atomic scattering factors used were taken from the International Tables[8].

The iodine and iron positions were readily located from the three-dimensional Patterson function[9], and the remaining nonhydrogen atoms were located from difference Fourier maps. The structure was found to contain two crystallographically distinct tri–iodide anions located around the crystallographic centres of symmetry at 0,0,0 and ½,0,0.

The structure was refined by least-squares using isotropic temperature factors for all atoms. This refinement converged at $R_1=12.1\%$ and $R_2=13.7\%$. The refinement was then continued using anisotropic temperature factors for the iodine and iron atoms until $R_1=6.5\%$ and $R_2=8.9\%$. At this stage, a difference Fourier was calculated using only those reflections with $\sin\theta/\lambda$ less than 0.35 Å^{-1} in an attempt to locate the hydrogen atoms. Although in most cases this map showed peaks of about 0.8e. Å^{-3} at the points where hydrogen atoms were expected, there was also a large number of peaks of the same magnitude that could not be assigned to hydrogen atoms or to resiual density at the heavy–atom sites. The methyl hydrogens could not be located. Nevertheless, in subsequent refinement cycles, the eight hydrogens on the cyclopentadienyl rings were included in calculated positions with C–H=0.9 Å. This C–H distance, though short in comparison with spectroscopic results, is in accordance with the results from numerous X–ray studies[10]. The hydrogen parameters were not refined. After inclusion of the H atoms, R_1 and R_2 were 6.5% and 8.7%, and a close examination of the data showed that for the strong, low order reflections, $|Fo|$ was considerably less than $|Fc.|$ To correct this, Zachariasen's formulation of the extinction problem was adopted [11], and his extinction parameter was refined as a variable in the next least-squares cycle.[12]

The resulting value of the extinction parameter was $4.9(2)\times10^{-6}$ for intensities on an absolute scale, and the residuals were considerably reduced to $R_1=3.8\%$ and $R_2=5.7\%$. Such a large decrease in the residuals was not expected. However, it is likely that our «extinction» correction also supplies an approximation to the θ–dependent component of the absorption correction that was neglected in our empirical absorption correction.

The contribution to the least-squares residual was then calculated for various classes of reflections based on $|Fo|$, $\sin\theta/\lambda$, and the Miller indices. No systematic variation of the residuals was found indicating that the weighting scheme was satisfactory. The standard deviation of an observation of unit weight was 3.12, and a difference Fourier map showed no peaks greater than 0.7 e.Å^3 in height.

In those cases where no crystallographic symmetry is imposed on the tri-iodide anion, two unequal I–I distances have been reported.[13,14] Therefore we next attempted to refine two models containing asymmetric tri-iodide anions with 50:50 disorder around the centres of symmetry. Model 1 retained atoms I_2 and I_4 in the positions found from the refinement of the symmetric ion model, but I_1 and I_3 were displaced from the centres of symmetry by 0.1 Å in the directions of the I–I bonds.

In model 2 atoms I_1 and I_3 were retained at the centres of symmetry, but I_2 and I_4 were each replaced by two half atoms, I_{2A}, I_{2B} and I_{4A}. I_{4B} respectively, displaced by + and –0.1 Å from the symmetrically refined positions, along the I–I bonds.

These models were refined by full matrix least-squares techniques and, in view of the expected high correlation between the disordered atom parameters, only half of the calculated shifts were applied for these parameters.

Refinement of model 1 resulted in I_1 and I_3 returning to the centric sites, and a singular least-squares matrix was obtained after one cycle. Refinement of model 2, however, resulted in a small increase in the separation of the disordered sites and in spite of the correlation (around 99%) between the disordered atom parameters this refinement reduced the residuals to $R_1=3.5\%$ and $R_2=5.7\%$ in two cycles. All of the atomic vibration parameters remained physically reasonable. In order to be certain that the refinement had truly converged, we calculated another three cycles of refinement for model 2. No further change in the residuals was found, and the maximum calculated (full) shift in the last cycle was less than one half of the corresponding standard deviation. According to Hamilton's R ractor ratio test,[15] the disordered model 2 fits the diffraction data significantly better than the ordered centro-symmetric model. Moreover, the distances between the disordered site positions after convergence, 0.23(4) and 0.26(5) Å, differ significantly from zero. (The standard deviations of these quantities, in common with all such quantities in this paper, are calculated with parameter correlation and cell parameter errors taken into account.)

We therefore have evidence that the tri-iodide ion is asymmetric in this structure at room temperature. None of the parameters of the cation atoms changed significantly on changing from the ordered to the disordered model.

At this, the final stage, the standard deviation of an observation of unit weight was 2.96, and a difference Fourier map showed no peaks greater than 0.6 e. Å^{-3} in height.

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(7) J.A. Ibers and W.C. Hamilton, *Acta Cryst.*, *17*, 781, (1964).
(8) International Tables for X-ray Crystallography, Vol. III, Kynoch Press, Birmingham, England, 1962.
(9) The programs used in this work were local modifications of Zalkin's FORDAP Fourier summation program, J.A. Ibers' NUCLS least-squares refinement program, Busing and Lev's ORFEE function and error program, and Johnson's ORTEP thermal ellipsoid plotting program.
(10) W.C. Hamilton and J.A. Ibers, « Hydrogen Bonding in Solids », W.A. Benjamin Inc., New York, 1968.
(11) W.H. Zachariasen, *Acta Cryst.*, *23*, 558 (1968).
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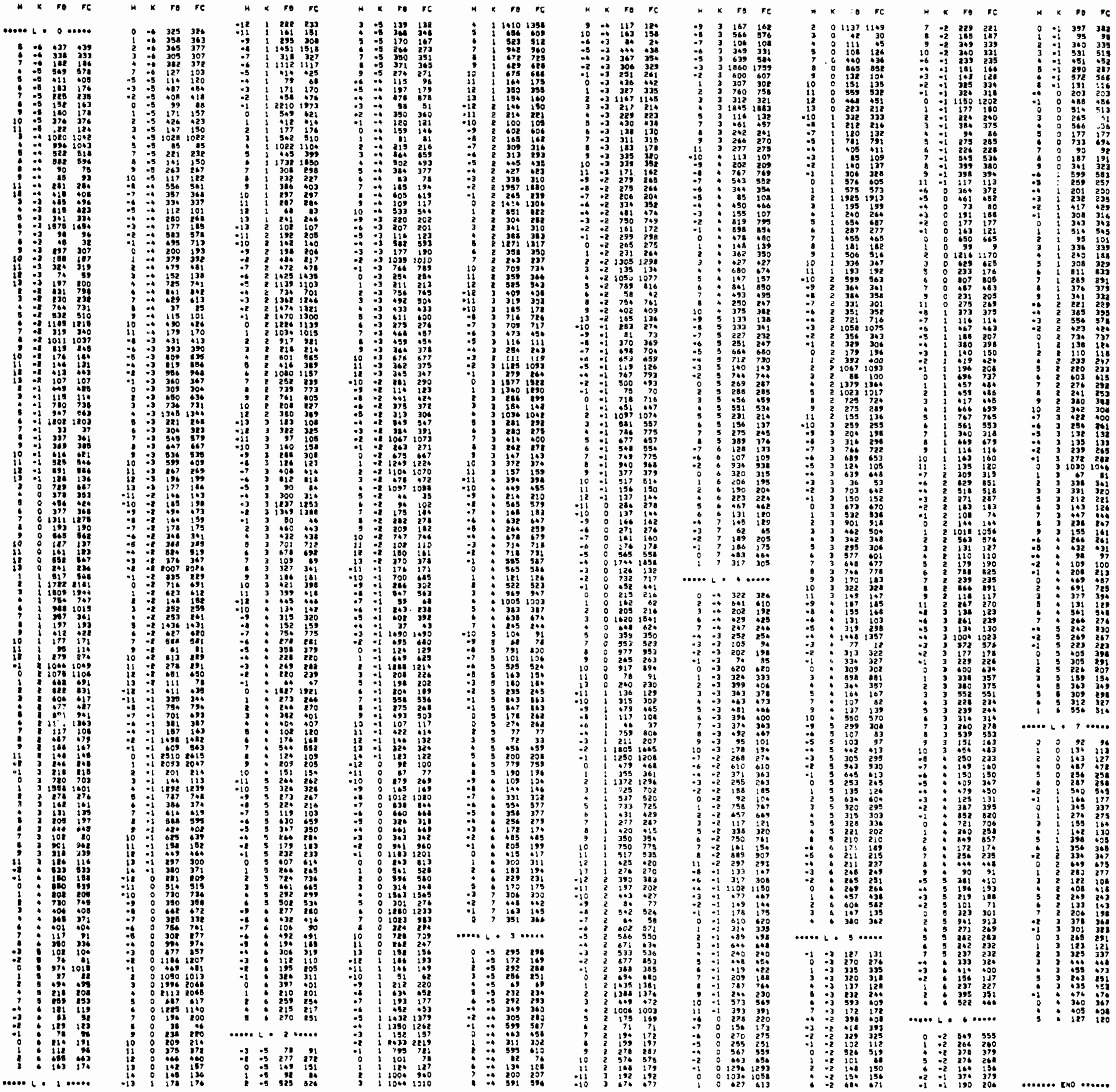
Table I. Observed and Calculated Structure Amplitudes (Electrons x 10) for 1,1'-Dimethylferricenium tri-iodine.



A listing of the final values of $|Fo|$ and $|Fc|$ in electrons X 10, is given in Table I, an dthe final least-squares parameters, together with their standard deviations, are given in Tables IIa and IIb.

Description of the Structure

The crystal structure is built up by the packing of well-separated $(C_6H_7)_2Fe$ cations and I_3 anions. There are no Fe–I distances in the structure of less than 4.7 Å. A projection of the structure down the *b* axis and the atomic numbering are shown in Figure 1. Listings of selected interatomic distances and angles are given in Tables III and IV. Table V gives details of the weighted best least-squares planes through the cyclopentadienyl rings as found by the method of Hamilton.[16]

The tri-iodide anion. It has long been recognized that the structure of the tri-iodide anion appears to depend on its environment in a crystal lattice. The results for a number of compounds containing the I_3^- species have been summarized in Table VI. For cases where the ion lies at a symmetry element in the structure, equal I–I distances have been reported, but

[16] W.C. Hamilton, *Ibid.*, *18*, 502 (1965).
[17] J. Trotter and A.C. MacDonald, *id.*, *21*, 359 (1966).

Table IIa. Final least-squares parameters for 1,1'-dimethylferricenium tri-iodide.

Atom	x	y	z	B
I1	0	0	0	—[a]
12A	0.1495(17)[b]	—0.0488(30)	0.1912(27)	—
12B	—0.1647(17)	0.0390(26)	—0.1762(24)	—
I3	0.5	0	0	—
I4A	0.5769(18)	—0.2070(44)	—0.2121(30)	—
I4B	0.4230(17)	0.1914(41)	0.2521(30)	—
Fe	0.7268(1)	0.4200(2)	0.3165(2)	—
CA1[c]	0.8521(7)	0.3378(15)	0.2240(14)	3.6(2)
CA2	0.7793(7)	0.1712(15)	0.3239(14)	3.6(2)
CA3	0.7028(8)	0.1895(17)	0.2338(16)	4.6(2)
CA4	0.7265(9)	0.3620(18)	0.0860(16)	5.1(3)
CA5	0.8169(8)	0.4533(16)	0.0770(15)	4.4(2)
CA6	0.9456(9)	0.3751(19)	0.2719(17)	5.5(3)
CB1	0.7484(8)	0.5878(16)	0.4826(15)	4.1(2)
CB2	0.6809(8)	0.4187(17)	0.5805(15)	4.5(2)
CB3	0.6063(8)	0.4156(17)	0.4863(16)	4.7(2)
CB4	0.6284(9)	0.5880(18)	0.3293(16)	5.1(3)
CB5	0.7144(8)	0.6863(17)	0.3340(16)	4.9(3)
CB6	0.8360(9)	0.6442(20)	0.5408(18)	6.0(3)

[a] These atoms were refined with anisotropic temperature factors See Table IIb. [b] Figures in parentheses here and in succeeding tables are the estimated standard deviations in the least significant digits. [c] The carbon atoms are numbered such that CA1 is the carbon in ring A attached to CA6, the methyl group. (Fig. 1).

Table IIb. Anisotropic Thermal Parameters for the Heavy Atoms.

Atom	β_{11}[a]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
I1	0.00827(9)	0.0181(3)	0.0164(3)	0.0020(1)	—0.0022(1)	—0.0069(2)
12A	0.0076(5)	0.034(2)	0.029(3)	0.0025(9)	—0.0065(9)	—0.010(1)
I2B	0.0091(8)	0.029(2)	0.017(1)	0.0069(9)	—0.0045(6)	—0.009(1)
I3	0.00449(7)	0.0242(3)	0.0181(3)	0.0003(1)	—0.0026(1)	—0.0037(2)
I4A	0.0069(3)	0.034(2)	0.020(3)	0.0035(5)	—0.0032(8)	—0.010(2)
I4B	0.0055(3)	0.032(2)	0.020(3)	0.0014(5)	—0.0019(8)	—0.011(2)
Fe	0.00435(4)	0.0167(4)	0.0143(4)	0.0028(2)	—0.0014(1)	—0.0071(3)

[a] The form of the anisotropic thermal ellipsoid is given by: $\exp.[-(\beta_{11}.h^2+\beta_{22}.k^2+\beta_{33}.l^2+2.\ \beta_{12}.h.k+2.\beta_{13}.h.l.+2.\beta_{23}.k.l.)]$.

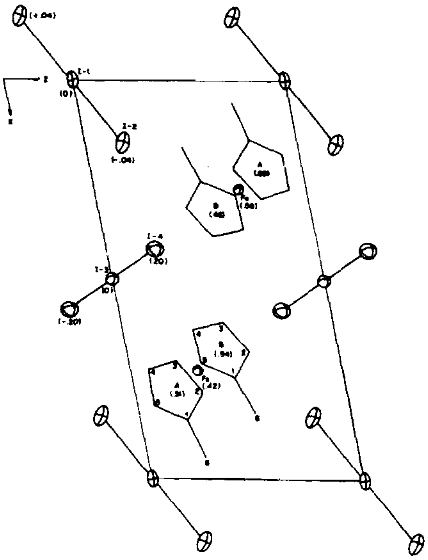


Figure 1. 1,1'-dimethylferricenium tri-iodide - projection along b (y values in parentheses).

Table III. Selected Interatomic Distances (Å) in 1,1'-dimethylferricenium tri-iodide.

I2A-I2B	5.816(6)	I4A-I4B	5.849(6)
I1-I2A	2.85(2)	I3-I4A	2.81(3)
I1-I2B	2.97(2)	I3-I4B	2.97(3)
Fe-CA1	2.12(1)	Fe-CB1	2.13(1)
Fe-CA2	2.08(1)	Fe-CB2	2.11(1)
Fe-CA3	2.08(1)	Fe-CB3	2.06(1)
Fe-CA4	2.04(1)	Fe-CB4	2.05(1)
Fe-CA5	2.02(1)	Fe-CB5	2.04(1)
Fe-CA6	3.26(1)	Fe-CB6	3.27(1)
CA1-CA2	1.44(2)	CB1-CB2	1.40(2)
CA1-CA5	1.41(2)	CB1-CB5	1.37(2)
CA2-CA3	1.42(2)	CB2-CB3	1.42(2)
CA4-CA5	1.39(2)	CB4-CB5	1.39(2)
CA3-CA4	1.38(2)	CB3-CB4	1.42(2)
CA1-CA6	1.50(2)	CB1-CB6	1.49(2)
CA1-CB1	3.52(2)	CA6-CB6	3.72(2)
CA2-CB2	3.46(2)	CA5-CB5	3.40(2)
CA3-CB3	3.30(2)	CA4-CB4	3.26(2)

even within the same structure, independent estimates of the bond lengths differ by several standard deviations. Typical examples are 2.928(3) and 2.943(3) Å in modification I of $(C_2H_5)_4NI_3$,[14] and 2.907(2) and 2.925(3) Å in the present structure if the ion is assumed to be symmetric. When no crystallographic symmetry is imposed on the anion, invariably two significantly different I—I distances are found in the same ion.

For example, in modification II of $(C_2H_5)_4NI_3$ there are two independent I_3 anions in general positions. The distances are 2.912(4) and 2.961(4) Å for one ion and 2.892(4) and 2.981(4) Å for the other.[14]

Migchelsen and Vos have carried out electrostatic crystal field calculations[14] on a number of I_3^-—containing structures, and have shown a clear correlation between the electrostatic crystal field and the I—I bond lengths.

Table IV. Selected Interatomic Angles (°) in 1,1′-dimethylferricenium tri-iodide.

I2A-I1-I2B	176(1)	I4A-I3-I4B	175(1)
CA1-Fe-CA2	40.0(4)	CB1-Fe-CB2	38.5(4)
CA2-Fe-CA3	40.6(4)	CB2-Fe-CB3	39.9(5)
CA3-Fe-CA4	39.1(5)	CB3-Fe-CB4	40.1(5)
CA4-Fe-CA5	40.1(5)	CB4-Fe-CB5	39.6(5)
CA5-Fe-CA1	39.0(4)	CB5-Fe-CB1	38.1(4)
CA2-CA1-CA5	106(1)	CB2-CB1-CB5	106(1)
CA1-CA2-CA3	108(1)	CB1-CB2-CB3	109(1)
CA2-CA3-CA4	108(1)	CB2-CB3-CB4	107(1)
CA3-CA4-CA5	109(1)	CB3-CB4-CB5	106(1)
CA4-CA5-CA1	109(1)	CB4-CB5-CB1	112(1)
CA2-CA1-CA6	125(1)	CB2-CB1-CB6	126(1)
CA5-CA1-CA6	128(1)	CB5-CB1-CB6	129(1)
CA1-Fe-CB1	111.8(4)	CA4-Fe-CB4	107.1(5)
CA2-Fe-CB2	111.3(4)	CA5-Fe-CB5	111.0(5)
CA3-Fe-CB3	108.0(5)		

Table V. Weighted best least-squares planes through the cyclopentadienyl rings.

1) Plane 1 through CA1, CA2, CA3, CA4, CA5, CA6.
$5.376x - 5.781y - 5.840z - 1.315 = 0$ [a]

Deviations from the plane (Å)

CA1	0.006(11)	CA5	—0.003(12)
CA2	—0.012(11)	CA6	0.003(13)
CA3	0.015(12)	Fe	—1.685(1)
CA4	—0.006(13)		

2) Plane 2 through CB1, CB2, CB3, CB4, CB5, CB6.
$6.889x - 5.705y - 5.304z + 0.773 = 0$

Deviations from the plane (Å)

CB1	0.015(11)	CB5	0.008(12)
CB2	—0.001(12)	CB6	—0.013(13)
CB3	—0.004(13)	Fe	1.705(1)
CB4	—0.006(13)		

3) Angle between planes 1 and 2 = 6.6°.

[a] The quantities x, y, z, are fractional atomic coordinates.

Bernstein and Herbstein[4] reported finding evidence for disorder of asymmetric I_3 anions around a crystallographic symmetry site in the electron density maps of $(C_5H_5)_2FeI_3$, and suggested that at low temperature it might be possible to resolve the components of such a disorder. Our results show that even at room temperature it is possible (at least for this compound) to resolve the apparently symmetric I_3 anions into two equal asymmetric components with I—I distances of 2.86(2) and 2.98(2) Å. These distances are in good agreement with those found in cases where the electrostatic fields around the anions are highly asymmetric,[13,19,20,21] and our results can be interpreted as showing an equilibrium in I_3^- between the forms, $I^- \ldots I{-}I$ and $I{-}I \ldots I^-$. Also, since it is possible to resolve the two forms, it can be stated that the lifetime of each component must be at least longer than the time scale of the X-ray diffraction experiment ($\approx 10^{-18}$s, ref. 23).

In a symmetric environment, the crystal structure would be expected to contain a 50:50 mixture of the two forms, but in an asymmetric environment, the equilibrium should be displaced to one side or the other. Since the previously reported atomic positions for I_3^- are then at the weighted mean positions of the component I atoms, it follows that the reported I—I distances should vary as a function of the electrostatic crystal field, exactly as found by Migchelsen and Vos.

The 1,1′–dimethylferricenium Cation. Trotter and MacDonald[17] have used the mean angle subtended at the iron atom by pairs of almost superimposed atoms when a ferrocene system is projected on the mean plane of the two rings as a measure of the eclipsedness of the ring systems.

For an exactly eclipsed system this angle is 0°, and for a completely staggered system the angle is 36°. In the dimethylferricenium cation the mean angle is 2.2°. The rings are therefore in an eclipsed position.

Table VI. Distances Observed for tri-iodide anions.

Compound	I1 - I2	I2 - I3	Symmetry assumed	Reference
CsI_3	2.83(2)	3.04(2)	—	13
Cs_2I_8	2.83(2)	3.00(2)	—	19
NH_4I_3 [a]	2.791(4)	3.113(4)	—	20
	2.82	3.10	—	21
$(C_6H_5)_4AsI_3$	2.91(2)	2.91(2)	$\bar{1}$	22
$(C_2H_5)_4NI_3$ (I) [b]	2.928(3)	2.928(3)	2/m	14
	2.943(3)	2.943(3)	2/m	»
$(C_2H_5)_4NI_3$ (II)	2.912(4)	2.961(4)	m	»
	2.892(4)	2.981(4)	m	»
$(C_5H_5)_2FoI_3$	2.93(2)	2.93(2)	$\bar{1}$	4
$(C_5H_4CH_3)_2FeI_3$	2.907(2)	2.907(2)	$\bar{1}$ [c]	This Publication
	2.925(2)	2.925(2)	$\bar{1}$	»
	2.85(2)	2.97(2)	— [d]	»
	2.89(3)	2.97(3)	—	»

[a] Two independent estimates by different workers. [b] Two different crystal modifications each containing two independent tri-iodide anions. [c] Assuming no disorder. [d] Assuming 50:50 disorder cf asymmetric ions.

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(23) E.L. Muetterties, *Inorg. Chem.*, *4*, 769 (1965).

Moreover, the methyl groups lie adjacent to each other. The symmetry of the cation is thus close to C_{2v}.

Although the mesomeric properties of the methyl groups might be expected to affect the electron densities in the ring π systems, we find no systematic variation of the C–C distances. In the two rings, the C–C distances vary from 1.36(2) to 1.44(2) Å, with a mean of 1.40(1) Å. The mean distance is in good agreement with that of 1.40 Å found from X-ray work on ferrocene,[3] although longer distances of up to 1.44 Å have been obtained for the latter parameter from electron-diffraction measurements.[18]

The individual ring systems, together with the methyl groups, are both planar within 0.015 Å, but the planes of the rings are not parallel. The best least-squares planes through the atoms of the two rings are inclined at 6.6° to one another. This is probably due to non-bonded interaction between the methyl groups. Consideration of the inter-ring C–C distances shows that the interplane angle can be regarded as being due to a rotation of 3.3° of each ring about the C_3–C_4 vector so as to increase the separation of the methyl groups. In the configuration found the inter-ring distances increase smoothly from 3.30 (2) Å for the C_3–C_4 bond separation to 3.42 Å for the separation of the C_2–C_5 vector, to 3.52 Å for the C_1 separation, to 3.72 Å for the CH_3–CH_3 distance. Assuming C_{2v} symmetry for the cation, the mean Fe–C distances also increase on going from the C_3–C_4 end of the ring to the C_1 end. The mean of the Fe–C_4 distances is 2.04(1) Å, the mean of the Fe–C_2 and FeC_5 distances is 2.08(1) Å, and the mean Fe–C_1 distance is 2.13(1) Å. This trend may be interpreted as being simply a consequence of the tilt of the rings, or alternatively, as being due to a higher concentration of electron density in the C_2, C_3, C_4, C_5 ends of the rings owing to the electron-releasing power of the methyl groups.

The Fe-ring perpendicular distances are 1.69 and 1.70 Å. As predicted by Prins,[2] these are longer than in ferrocene (1.66 Å). However, the distances found are very much shorter than the value 1.93 Å estimated by Prins. In addition, since we have found here a clear indication of steric interaction between the methyl groups, a somewhat shorter distance might be expected to be found in unsubstituted ferricenium, or even in a staggered form of dimethylferricenium. In this light the distance of 1.65 Å reported by Bernstein and Herbstein[4] seems very reasonable.

Thus it appears that the metal-to-ring distance in the ferricenium cation is practically the same as in ferrocene, despite the difference in stability between the two species.