and at any reasonable distance from the sulfur atom it would be much too close to the axial hydrogens of the adjacent complex cation. Oxygen–hydrogen distances of about 1 Å would be required to achieve this orientation.

The ring conformation is $\delta\delta\delta$ in the $Ni(en)_3^{2+}$ ion and both Λ and Δ enantiomers must be present in the centric cell. The hydrogen bonding is extensive and differs in one respect from that previously proposed for the $\delta\delta\delta$ conformation.[7] For any one of the disordered sulfate orientations five of the six axial as well as five of the six equatorial amine hydrogens are at hydrogen-bonded distances from sulfate oxygens. A drawing of the unit cell with just one sulfate orientation and all the associated hydrogen bonds is shown in Figure 2. Raymond, Corfield, and Ibers[7] have suggested that no more than one of the axial hydrogens at either end of the cation can form a hydrogen bond in the $\delta\delta\delta$ conformation. This is certainly true when the two H-bond acceptors are constrained by van der Waals forces to be no closer than 3 Å or so, but in this case the two acceptors are sulfate oxygens and are only 2.5 Å apart. By orienting the sulfate group as it occurs in this structure it is possible to form H bonds to three axial hydrogens in one neighboring cation and two axial hydrogens in the other. The disorder of the sulfate group will vary the orientation of the H-bond pattern, but the basic pattern will be the same for any of the disordered positions of the anion.

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Crystal and Molecular Structure of Diacetylferrocene

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Diacetylferrocene crystallizes as orange needles in the monoclinic space group $P2_1/c$ with $a = 5.898 \pm 0.002$ Å, $b = 13.036 \pm 0.005$ Å, $c = 14.962 \pm 0.006$ Å, and $\beta = 90.68 \pm 0.04°$. There are four molecules per unit cell; $d_c = 1.559 \pm 0.002$ g/cm^3 and $d_m = 1.54 \pm 0.01$ g/cm^3. The structure was refined by full-matrix least-squares methods with anisotropic thermal parameters to a final R of 6.7% for the 2570 observed reflections measured using an automatic diffractometer with molybdenum radiation. The cyclopentadienide rings are planar and parallel with an average C–C distance 1.426 ± 0.014 Å. The acetyl groups are in the 1,3′ configuration with an average rotation of 4° 4′ of the rings from the eclipsed configuration.

Introduction

The dependence of the configuration of ferrocene derivatives on the nature of substituents on the cyclopentadienide (Cp) rings is obscure. Although the relationship between the angle of rotation of the Cp rings about their centers and intermolecular forces has been discussed,[1–3] no definitive conclusions were reached. In fact, although only van der Waals interactions exist between molecules in ferrocenedicarboxylic acid, the Cp rings are almost completely eclipsed.[4] However, the eclipsed configuration may be rationalized in terms of the dimerlike molecules formed by hydrogen bonding between carboxylic acid groups from two molecules. Therefore, an investigation of diacetylferrocene was undertaken since hydrogen bonding between molecules is not possible for this compound. The results provide information regarding the preferred configuration of substituted ferrocenes and the relationship between the rotation of the Cp rings and intermolecular forces.

Experimental Section

Diacetylferrocene was purchased from Alfa Inorganics. The crystals are orange needles elongated along $\tilde{a}$. Preliminary Weissenberg photographs taken about $\tilde{a}$ revealed that the crystals were monoclinic. The systematic absences of $h0l$ for $l = 2n + 1$ and $0k0$ for $k = 2n + 1$ indicated that the space group was $P2_1/c$ (C_{2h}^5).

One well-developed needle was cleaved with a razor blade to give a crystal (0.176 × 0.110 × 0.065 mm parallel to $\tilde{a}$, $\tilde{b}$, and $\tilde{c}$, respectively) which was mounted on a glass fiber. The fiber and crystal were dipped into liquid nitrogen and then mounted on a General Electric single-crystal orienter. The $\tilde{b}$ axis was parallel to the ϕ axis of the orienter. The unit cell dimensions were determined using a narrow beam of molybdenum radiation ($\lambda(\alpha_1)$ 0.70926 and $\lambda(\alpha_2)$ 0.71354 Å). The average of these measurements were $a = 5.898 \pm 0.002$ Å, $b = 13.036 \pm 0.005$ Å, $c = 14.962 \pm 0.006$ Å, and $\beta = 90.68 \pm 0.04°$. The density calculated for four molecules per unit cell is 1.559 ± 0.002 g/cm^3; the density determined by flotation is 1.54 ± 0.01 g/cm^3.

The intensity measurements were made with a scintillation counter using a wide beam of molybdenum radiation (takeoff angle of 3.7°). A linear amplifier–pulse height selector combination together with a zirconium filter at the counter window

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(1) J. Trotter and A. C. MacDonald, *Acta Crystallogr.*, **21**, 359 (1966).

(2) M. R. Churchill and R. Mason, *Advan. Organometal. Chem.*, **5**, 93 (1967).

(3) M. R. Churchill and J. Wormald, *Inorg. Chem.*, **8**, 716 (1969).

(4) G. J. Palenik, *ibid.*, **8**, 2744 (1969).

was employed to eliminate the noncharacteristic radiation. The diffractometer was controlled by a prepunched paper tape. The stationary counter–stationary crystal technique was employed in measuring 4125 reflections with $2\theta \leq 60.0°$. A 20-sec count was taken for each reflection. Four standard reflections were counted periodically with 46 measurements of each standard being made during the course of the intensity measurements. The root-mean-square deviation for each of the four reflections was about 2% with no apparent trend with time. Reflections of the type $h0l$ with $l = 2n + 1$, required by the space group to be absent, were also measured. Those absent reflections which were not on a radiation streak were used to derive an empirical background curve. Of the 3371 unique reflections with $2\theta \leq 60°$, only the 2570 reflections whose intensities were greater than 1.2 times the background count were considered to be observed reflections and were used in the structure analysis. No correction for the $\alpha_1 - \alpha_2$ splitting was made since the doublet could be measured under the experimental conditions employed. The linear absorption coefficient (μ) for the crystal with Mo Kα radiation is 13.2 cm^{-1}. Since the value of μt only varies from 0.09 to 0.23, no absorption corrections were made. The reduction of these data to a set of observed amplitudes on an arbitrary scale was carried out in the usual manner.

Determination and Refinement of the Structure

The position of the iron atom was deduced from a sharpened three-dimensional Patterson function with the origin peak removed. However, the x and z coordinates were approximately $^1/_4$, making direct use of the heavy-atom method difficult. A minimum Patterson function based on the Fe–Fe vector was computed. The positions of the carbon atoms of one ring and the attached carbon atom were located from the minimum function. The remaining light atoms were located in subsequent Fourier syntheses. The structure was refined by full-matrix least-squares methods using individual isotropic thermal parameters to an R of 9.1% and with anisotropic thermal parameters to an R of 7.6%.

A difference Fourier synthesis was computed to locate the hydrogen atoms. The hydrogen atoms on the Cp rings were well resolved; however, the methyl hydrogen positions were ill defined. The 14 hydrogen atoms were included in the structure factor calculation (with an isotropic thermal parameter equal to the value +1.0 obtained from the isotropic refinement for the atom to which the hydrogen atom is bonded) but their parameters were not refined. Two least-squares cycles reduced R to 6.7% and the refinement was terminated. The final position parameters are given in Table I and the final thermal parameters in Table II. A final difference Fourier synthesis was computed without including the hydrogen atom contributions and a new set of hydrogen atom positions was determined. The final hydrogen atom positions and their thermal parameters are given in Table III. The observed and calculated (using the parameters in Tables I–III) structure factors are given in Table IV.

In all the above calculations the scattering factors for Fe, O, and H were from ref 5. For the carbon atoms, the graphite curve given by McWeeny[6] was used.

TABLE I

THE FINAL POSITIONAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS[a]

Atom	x (σ_x)	y (σ_y)	z (σ_z)
C*R*1	2393 (8)	−1086 (3)	3184 (3)
C*R*2	3686 (8)	−1185 (4)	2366 (3)
C*R*3	2202 (10)	−0969 (4)	1648 (3)
C*R*4	0029 (9)	−0721 (4)	1988 (4)
C*R*5	0112 (7)	−0811 (4)	2931 (3)
C*A*1	3359 (8)	−1171 (4)	4094 (3)
C*M*1	1730 (12)	−1204 (7)	4844 (4)
O*A*1	5398 (7)	−1245 (4)	4215 (3)
C*R*6	3765 (8)	1448 (3)	1808 (3)
C*R*7	5085 (8)	1256 (4)	2591 (3)
C*R*8	3657 (10)	1384 (4)	3346 (3)
C*R*9	1463 (10)	1664 (4)	3022 (4)
C*R*0	1505 (8)	1696 (4)	2082 (4)
C*A*2	4576 (9)	1328 (4)	0890 (4)
C*M*2	2875 (12)	1383 (5)	0140 (4)
O*A*2	6575 (7)	1192 (4)	0734 (3)
Fe	24001 (10)	02662 (5)	25028 (4)

[a] All values $\times 10^{+4}$ except for the iron atom which is $\times 10^{+5}$.

TABLE II

FINAL THERMAL PARAMETERS WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES[a]

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C*R*1	198 (12)	30 (2)	35 (2)	−8 (8)	2 (8)	6 (4)
C*R*2	235 (13)	30 (2)	36 (2)	14 (9)	44 (9)	3 (4)
C*R*3	301 (16)	38 (3)	29 (2)	−46 (10)	3 (9)	−15 (4)
C*R*4	255 (15)	48 (3)	33 (2)	−68 (11)	−34 (9)	1 (4)
C*R*5	176 (11)	33 (2)	38 (2)	−34 (8)	15 (8)	2 (4)
C*A*1	220 (13)	44 (3)	33 (3)	−2 (10)	20 (8)	10 (4)
C*M*1	317 (19)	112 (6)	38 (2)	34 (18)	23 (12)	24 (7)
O*A*1	223 (11)	85 (3)	45 (2)	20 (10)	−22 (7)	30 (4)
C*R*6	228 (12)	27 (2)	30 (2)	−22 (8)	−10 (8)	18 (3)
C*R*7	175 (11)	37 (2)	38 (2)	−24 (8)	−20 (8)	4 (4)
C*R*8	318 (17)	41 (3)	30 (2)	−43 (11)	−17 (9)	−15 (4)
C*R*9	281 (16)	38 (3)	42 (2)	15 (11)	29 (10)	−4 (4)
C*R*0	218 (13)	30 (2)	41 (2)	22 (9)	−8 (8)	5 (4)
C*A*2	236 (14)	35 (2)	40 (21)	−19 (10)	9 (9)	10 (4)
C*M*2	385 (12)	65 (4)	30 (2)	−10 (14)	−8 (10)	4 (5)
O*A*2	263 (12)	91 (4)	44 (2)	14 (11)	38 (8)	3 (4)
Fe	1543 (19)	294 (4)	262 (3)	−70 (12)	−54 (10)	16 (5)

[a] The temperature factor is of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$. The values are multiplied by 10^{+4} except for the iron atom which is multiplied by 10^{+5}.

TABLE III

PROBABLE HYDROGEN POSITIONS[a]

Atom	x	y	z	B, Å^2	Distance, Å
H2 (C*R*2)	530	−141	234	4.38	1.00
H3 (C*R*3)	274	−076	099	4.65	1.08
H4 (C*R*4)	−134	−056	169	4.83	0.94
H5 (C*R*5)	−106	−064	337	3.96	0.99
H11 (C*M*1)	−001	−100	485	7.32	1.06
H12 (C*M*1)	212	−113	521	7.32	0.60
H13 (C*M*1)	190	−210	504	7.32	1.21
H7 (C*R*7)	668	111	254	4.16	0.97
H8 (C*R*8)	378	119	403	4.83	1.06
H9 (C*R*9)	028	168	356	5.14	1.07
H10 (C*R*0)	009	185	178	4.29	0.97
H21 (C*M*2)	335	166	−032	6.03	0.82
H22 (C*M*2)	268	187	008	6.03	0.65
H23 (C*M*2)	177	123	051	6.03	0.88

[a] The hydrogen atom is given followed by the atom to which it is bonded (in parentheses), the position parameters $\times 10^3$, the isotropic thermal parameter used in the calculations, and the corresponding C–H distance.

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(5) "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1962.

(6) R. McWeeny, *Acta Crystallogr.*, **4**, 513 (1951).

TABLE IV

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(CH_3COC_5H_4)_2Fe^a$

H= 0,K= 0		
2	1294	-1596
4	1137	1226
6	673	-725
8	169	166
10	181	-191
12	652	669
14	309	-274
16	254	220
18	243	-221
20	128	110
H= 1,K= 0		
0	484	-481
2	218	-202
4	491	484
6	615	602
8	93	-74
10	37	13
12	273	-276
14	-23	15
16	57	38
18	-19	-6
20	54	34
-2	640	-630
-4	131	126
-6	654	619
-8	32	32
-10	279	282
-12	333	-351
-14	61	68
-16	-19	-15
-18	-19	-0
-20	70	77
H= 2,K= 0		
0	801	-791
2	343	342
4	855	-833
6	302	309
8	563	-549
10	508	542
12	306	-308
14	285	300
16	204	-187
18	181	166
20	140	-117
-2	577	549
-4	528	-530
-6	36	45
-8	547	-551
-10	314	311
-12	484	-494
-14	315	300
-16	209	-197
-18	-20	25
-20	56	-38
H= 3,K= 0		
0	62	-10
2	-19	-15
4	205	-209
6	80	67
8	-21	-24
10	152	163
12	63	-67
14	53	54
16	-19	-16
18	-21	-1
-2	196	197
-4	181	-166
-6	143	138
-8	301	-310
-10	48	28
-12	38	-27
-14	53	46
-16	66	-52
-18	67	65
H= 4,K= 0		
0	473	488
2	238	-245
4	622	605
6	410	-407
8	217	208
10	366	-391
12	182	170
14	130	-145
16	156	167
18	167	-171
-2	718	-710
-4	323	317
-6	347	-344
-8	486	498
-10	125	-104
-12	295	264
-14	224	-213
-16	136	133
-18	96	-76
H= 5,K= 0		
0	196	191
2	390	-378
4	109	-110
6	99	93
8	-22	14
10	58	51
12	-19	20
14	123	-131
16	-22	0
-2	75	-76
-4	324	325
-6	-23	12
-8	49	-25
-10	136	-133
-12	-19	33
-14	30	8
-16	104	96
H= 6,K= 0		
0	56	-51
2	249	252
4	64	-73
6	164	146
8	236	-245
10	206	195
12	153	-154
14	180	174
-2	138	127
-4	258	-244
-6	115	113
-8	164	-155
-10	243	226
-12	157	-141
-14	114	127
H= 7,K= 0		
0	88	-99
2	79	71
4	-19	-58
6	90	96
8	68	-70
10	131	148
-2	88	93
-4	52	-44
-6	98	90
-8	78	-87
-10	113	106
H= 8,K= 0		
0	182	185
2	236	-205
4	147	146
-2	225	-207
-4	152	146
H= 0,K= 1		
1	98	-16
2	511	-538
3	45	-27
4	584	-614
5	121	15
6	181	-182
7	55	-19
8	168	185
9	57	-45
10	122	135
11	-21	-15
12	124	-128
13	-24	4
14	37	-36
15	-22	14
16	134	-128
17	40	13
18	34	-26
19	51	5
20	-21	1
21	-22	-7
H= 1,K= 1		
0	177	-179
1	1641	-1686
2	688	674
3	930	880
4	121	148
5	657	-672
6	163	-145
7	365	360
8	145	-160
9	530	-564
10	225	-220
11	323	345
12	58	85
13	437	-447
14	-23	15
15	228	220
16	-19	20
17	199	-187
18	-19	26
19	116	123
20	54	-56
-1	1530	1528
-2	47	-70
-3	1173	-1138
-4	547	-554
-5	419	441
-6	68	-45
-7	395	-412
-8	65	68
-9	426	443
-10	219	211
-11	332	-333
-12	48	-43
-13	458	473
-14	38	41
-15	253	-239
-16	94	-97
-17	198	170
-18	52	24
-19	116	-106
-20	-22	-7
H= 2,K= 1		
0	58	-50
1	179	-170
2	182	173
3	66	-45
4	212	-182
5	197	-183
6	399	409
7	-20	42
8	50	59
9	-20	10
10	84	83
11	66	75
12	134	129
13	-23	-41
14	-22	-54
15	-20	4
16	27	4
17	67	-60
18	79	70
19	-21	-2
20	-22	-34
-1	72	-61
-2	347	345
-3	70	-85
-4	-21	-38
-5	272	251
-6	236	236
-7	43	35
-8	31	-37
-9	-20	1
-10	89	-98
-11	49	56
-12	41	29
-13	133	-143
-14	50	-48
-15	-20	0
-16	46	-18
-17	52	50
-18	31	-8
-19	-21	-28
-20	56	-26
H= 3,K= 1		
0	206	-166
1	797	765
2	38	-29
3	363	-357
4	274	266
5	588	604
6	160	-158
7	448	-464
8	245	238
9	396	396
10	67	-69
11	325	-329
12	-23	-17
13	281	285
14	-19	1
15	159	-141
16	35	45
17	216	208
18	52	-43
19	160	-149
-1	440	-460
-2	28	15
-3	600	598
-4	262	251
-5	392	-413
-6	130	-128
-7	312	320
-8	210	209
-9	385	-370
-10	124	-147
-11	368	340
-12	38	10
-13	259	-245
-14	-20	-28
-15	244	220
-16	34	39
-17	115	-106
-18	-21	-14
-19	-22	29
H= 4,K= 1		
0	182	160
1	116	127
2	47	-45
3	87	-87
4	66	-60
5	-21	42
6	214	-204
7	74	86
8	107	-100
9	58	59
10	64	51
11	-22	-21
12	-20	3
13	46	34
14	-19	12
15	53	-48
16	-21	-12
17	-21	-13
18	58	-31
-1	166	-152
-2	37	-26
-3	143	149
-4	96	-92
-5	93	-110
-6	213	-214
-7	164	160
-8	82	-86
-9	128	-87
-10	51	53
-11	107	112
-12	49	24
-13	88	-71
-14	49	32
-15	33	36
-16	-20	-9
-17	101	-73
-18	72	-34
H= 5,K= 1		
0	72	-70
1	329	-302
2	95	-101
3	223	228
4	-24	23
5	272	-270
6	180	187
7	211	205
8	103	-95
9	246	-245
10	-19	21
11	194	195
12	77	-85
13	147	-151
14	-21	13
15	119	126
16	-21	11
-1	280	275
-2	153	-162
-3	357	-344
-4	71	-81
-5	252	240
-6	245	247
-7	265	-256
-8	100	-98
-9	166	180
-10	77	65
-11	198	-202
-12	85	-83
-13	161	146
-14	52	-35
-15	152	-155
-16	32	-3
H= 6,K= 1		
0	88	88
1	188	-180
2	-21	9
3	109	98
4	53	-54
5	68	-65
6	45	-35
7	47	35
8	31	-3
9	88	-86
10	67	46
11	116	105
12	-21	-0
13	83	-95
14	37	30
-1	155	157
-2	57	53
-3	149	-136
-4	62	62
-5	55	68
-6	57	-33
-7	71	-73
-8	49	-49
-9	33	36
-10	52	42
-11	107	-92
-12	-21	-3
-13	53	59
-14	34	47
H= 7,K= 1		
0	46	23
1	206	187
2	35	-25
3	177	-166
4	53	53
5	148	152
6	52	-18
7	117	-121
8	-21	36
9	129	134
10	72	-54
11	142	-135
-1	184	-189
-2	34	-24
-3	175	171
-4	-19	18
-5	140	-147
-6	31	1
-7	130	131
-8	-21	26
-9	102	-108
-10	32	21
-11	146	145
H= 8,K= 1		
0	34	-16
1	56	53
2	-21	18
3	35	-39
4	36	19
5	-22	24
-2	-22	6
-3	56	61
-4	34	-22
-5	35	-38
H= 0,K= 2		
0	981	959
1	334	-340
2	911	-962
3	301	281
4	732	711
5	261	-286
6	657	-688
7	203	178
8	501	516
9	201	-198
10	445	-461
11	182	174
12	359	356
13	122	-100
14	267	-260
15	104	100
16	208	203
17	93	-81
18	162	-153
19	51	27
20	113	121
H= 1,K= 2		
0	224	228
1	140	122
2	144	-153
3	467	-457
4	75	77
5	445	-411
6	84	83
7	55	54
8	51	-59
9	203	-192
10	-20	38
11	90	-102
12	-23	24
13	149	161
14	-23	-20
15	45	-39
16	-19	24
17	50	31
18	32	-2
19	-21	37
20	33	6
-1	674	-674
-2	160	-149
-3	243	-225
-4	-24	41
-6	48	-24
-7	320	-335
-8	-20	33
-9	157	-175
-10	-20	-5
-11	130	-145
-12	-23	1
-13	-24	37
-14	-23	-20
-15	-21	-20
-16	-19	1
-17	30	14
-18	-20	-25
-19	-21	3
-20	32	20
H= 2,K= 2		
0	648	-596
1	39	30
2	579	571
3	300	-277
4	544	-519
5	401	383
6	565	591
7	-20	-6
8	517	-525
9	-20	32
10	486	490
11	66	87
12	405	-398
13	135	-150
14	283	272
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7	140	-136
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8	620	640
9	502	-515
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9	130	-123
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7	294	-304
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11	181	-178
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15	164	-153
16	136	-146
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9	183	-180
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12	218	205
13	140	-143
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2	107	-106
3	79	-87
4	91	90
5	91	97
6	119	-109
7	113	-107
8	71	78
9	58	74
-1	67	-64
-2	107	-103
-3	78	74
-4	98	97
-5	66	-82
-6	125	-117
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-8	70	78
-9	56	-68
-10	87	-89
H= 8,K= 5		
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H= 0,K= 6		
0	316	322
1	498	-492
2	326	-332
3	512	546
4	341	369
5	511	-508
6	236	-253
7	463	476
8	246	268
9	348	-346
10	154	-156
11	251	255
12	138	137
13	223	-226
14	146	-144
15	170	168
16	102	102
17	134	-124
18	90	-83
19	99	110
H= 1,K= 6		
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1	52	-38
2	72	57
3	137	147
4	-20	-29
5	133	122
6	176	-184
7	-20	55
8	127	135
9	-22	9
10	86	-89
11	131	149
12	38	-42
13	129	-145
14	-20	24
15	-19	29
16	33	-27
17	32	-15
18	-21	-23
19	55	-39
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-2	83	76
-3	50	47
-4	85	65
-5	114	114
-6	42	-51
-7	104	117
-8	-20	0
-9	138	158
-10	58	-54
-11	-24	48
-12	36	52
-13	-22	20
-14	-20	-5
-15	-19	-17
-16	32	42
-17	-20	-0
-18	-21	15
-19	-21	-6
H= 2,K= 6		
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1	778	768
2	486	462
3	577	-587
4	429	-425
5	390	379
6	260	243
7	400	-406
8	152	-168
9	266	265
10	-24	26
11	298	-307
12	-22	14
13	326	327
14	70	58
15	197	-199
16	97	-96
17	131	132
18	93	108
19	126	-122
-1	622	-598
-2	314	303
-3	657	662
-4	446	-445
-5	360	-366
-6	245	248
-7	341	329
-8	206	-193
-9	317	-322
-10	153	152
-11	178	175
-12	77	-82
-13	193	-190
-14	70	67
-15	188	194
-16	105	-109
-17	89	-82
-18	68	81
-19	116	107
H= 3,K= 6		
0	230	-213
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3	40	29
4	135	-112
5	-21	-34
6	166	157
7	151	161
8	41	55
9	-24	-21
10	73	-81
11	-22	-27
12	91	94
13	-19	-2
14	32	-47
15	-19	-8
16	-21	3
17	-21	31
18	73	71
-1	171	-179
-2	229	224
-3	56	-57
-4	143	-127
-5	39	-59
-6	129	120
-7	115	-122
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-9	-24	-0
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-16	30	-6
-17	69	-69
-18	-22	31
H= 4,K= 6		
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3	203	204
4	155	160
5	155	-164
6	290	-293
7	72	102
8	251	266
9	105	-124
10	205	-195
11	235	240
12	156	154
13	140	-145
14	99	-90
15	132	142
16	-21	55
17	75	-88
-1	314	311
-2	-23	12
-3	198	-197
-4	159	163
-5	107	109
-6	269	-272
-7	69	-83
-8	289	297
-9	114	122
-10	205	-216
-11	216	-206
-12	154	145
-13	154	132
-14	66	-73
-15	144	-136
-16	69	60
-17	36	67
H= 5,K= 6		
0	42	-48
1	90	-102
2	-23	6
3	86	84
4	38	17
5	112	-103
6	62	-58
7	68	83
8	60	41
9	115	-119
10	78	-59
11	34	36
12	52	25
13	-21	-50
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15	-22	16
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-2	-23	8
-3	152	-155
-4	-22	-14
-5	162	157
-6	30	-57
-7	119	-124
-8	44	51
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-11	66	-79
-12	66	59
-13	90	84
-14	31	-40
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H= 6,K= 6		
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1	211	207
2	113	94
3	198	-202
4	94	-102
5	163	149
6	97	99
7	140	-137
8	89	-82
9	100	100
10	-21	66
11	122	-118
12	58	-61
-1	220	-224
-2	82	89
-3	207	193
-4	127	-122
-5	156	-152
-6	153	138
-7	112	114
-8	98	-97
-9	122	-131
-10	50	47
-11	148	147
-12	71	-37
-13	87	-107
H= 7,K= 6		
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1	52	58
2	-21	38
3	-21	-36
4	-21	-45
5	31	32
6	-21	27
7	-21	-28
8	-22	0
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-2	51	40
-3	78	73
-4	-21	-18
-5	-21	-61
-6	-21	25
-7	70	59
-8	33	-42
-9	-22	-3
H= 0,K= 7		
1	102	29
2	235	241
3	105	115
4	248	257
5	49	41
6	114	65
7	49	-46
8	101	-85
9	65	73
10	138	-135
11	-24	3
12	84	88
13	33	-5
14	33	-11
15	48	29
16	83	84
17	42	13
18	-21	20
19	-22	-17
H= 1,K= 7		
0	1096	-1066
1	462	-454
2	616	590
3	284	286
4	722	-748
5	242	-228
6	448	442
7	41	68
8	204	-216
9	120	-132
10	340	355
11	-23	-0
12	296	-297
13	125	-121
14	199	205
15	30	49
16	203	-196

TABLE IV (*Continued*)

17	79	-80
18	154	142
19	57	52
-1	380	357
-2	843	817
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-4	312	-337
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-6	369	365
-7	72	-81
-8	299	-307
-9	135	156
-10	128	126
-11	106	-115
-12	286	-302
-13	204	211
-14	214	224
-15	92	-84
-16	119	-125
-17	78	71
-18	110	113
-19	-22	-7
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1	74	52
2	139	141
3	66	-76
4	47	-46
5	145	-153
6	155	-148
7	58	75
8	-23	9
9	-24	-29
10	49	-52
11	-23	-29
12	-21	-17
13	68	64
14	-19	-4
15	-19	-38
16	31	7
17	-21	-49
18	-22	-32
-1	122	-114
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-3	59	-68
-4	105	-95
-5	70	78
-6	98	-107
-7	-22	-41
-8	-23	21
-9	-24	-14
-10	-24	-19
-11	-23	42
-12	56	67
-13	94	-88
-14	-19	0
-15	34	-10
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-17	-21	7
-18	32	40
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0	474	458
1	132	139
2	310	-303
3	90	-106
4	300	284
5	300	291
6	276	-259
7	180	-191
8	172	177
9	154	163
10	252	-258
11	72	-75
12	230	242
13	74	79
14	171	-172
15	31	-37
16	126	124
17	84	100
-1	-21	-8
-2	389	-393
-3	174	170
-4	238	244
-5	126	-133
-6	256	-255
-7	110	125
-8	266	268
-9	121	-122
-10	224	-225
-11	46	42
-12	276	272
-13	-19	-24
-14	193	-188
-16	109	108
-17	-21	-44
-18	59	-53
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1	41	33
2	130	-135
3	-24	15
4	89	78
5	-23	21
6	88	94
7	-23	32
8	76	66
9	-20	0
10	44	-43
11	-19	10
12	35	20
13	-20	-0
14	51	-66
15	53	-25
16	35	37
-1	-24	-27
-2	148	-163
-3	63	67
-4	205	210
-5	48	-54
-6	-23	11
-7	67	66
-8	103	121
-9	33	35
-10	76	-79
-11	-19	0
-12	33	15
-13	-19	7
-14	-21	-44
-15	-21	14
-16	34	50
H= 5,K= 7		
0	235	-131
1	-22	-27
2	232	239
3	-21	26
4	230	-224
5	112	-112
6	109	121
7	81	76
8	174	-196
9	77	-77
10	235	222
11	32	43
12	124	-124
13	31	-35
14	153	135
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-2	300	296
-3	91	-75
-4	185	-179
-5	97	108
-6	77	75
-7	154	-164
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-9	94	98
-10	156	162
-11	78	-77
-12	123	-123
-13	-21	33
-14	164	161
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2	75	81
3	33	38
4	-19	-7
5	-19	-17
6	79	58
7	-20	7
8	30	-35
9	-21	-21
10	-21	28
11	57	36
12	38	-61
-1	30	23
-2	50	39
-3	31	-33
-4	111	-114
-5	34	10
-6	88	91
-7	-20	-30
-8	51	-32
-9	-21	27
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-11	55	-59
-12	58	-79
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0	109	114
1	91	92
2	118	-120
3	81	-74
4	94	83
5	33	48
6	106	-98
7	-22	-24
-1	67	-72
-2	109	-118
-3	68	68
-4	119	125
-5	31	-44
-6	94	-104
-7	-22	28
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1	977	-1008
2	87	44
3	819	641
4	105	93
5	351	-366
6	305	-292
7	186	191
8	129	124
9	192	-195
10	116	-135
11	220	230
12	328	329
13	273	-282
14	118	-103
15	177	173
16	32	35
17	135	-146
18	32	-34
H= 1,K= 8		
0	626	-570
1	171	-159
2	298	280
3	130	118
4	-20	19
5	50	-66
6	152	157
7	-22	-20
8	92	92
9	-24	33
10	108	-118
11	-23	-46
12	44	-64
13	-19	37
14	28	-15
15	35	-6
16	31	26
17	-21	-9
18	-22	7
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-2	80	75
-3	138	-135
-4	37	-53
-5	-20	30
-6	169	180
-7	-22	-10
-8	97	111
-9	-24	-22
-10	-23	5
-11	74	74
-12	91	-91
-13	67	-82
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-15	34	20
-16	31	-12
-17	-21	12
-18	32	57
H= 2,K= 8		
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2	100	93
3	410	-407
4	155	-174
5	364	367
6	-23	-29
7	327	-313
8	-24	-31
9	320	336
10	66	59
11	260	-259
12	-20	1
13	234	245
14	65	60
15	141	-140
16	-21	-47
17	136	140
18	36	53
-1	465	-453
-2	152	150
-3	427	432
-4	83	-81
-5	282	-277
-6	169	-149
-7	233	249
-8	-24	-12
-9	312	-309
-10	74	-84
-11	299	310
-12	38	-19
-13	288	-292
-14	32	17
-15	205	188
-16	-21	-34
-17	92	-97
-18	-22	-16
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1	-22	47
2	39	-52
3	-23	-34
4	59	-62
5	52	63
6	-24	7
7	-23	-9
8	-23	39
9	37	45
10	-21	32
11	69	-64
12	28	6
13	-19	32
14	-20	5
15	-21	-31
16	-21	-20
17	-22	-0
-1	38	-62
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-3	79	82
-4	36	-58
-5	67	-75
-6	-24	47
-7	95	114
-8	80	-89
-9	-22	-48
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-11	-19	31
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-13	33	8
-14	33	9
-15	-21	19
-16	31	-25
-17	35	-35
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3	219	223
4	172	175
5	286	-290
6	120	-116
7	219	216
8	39	12
9	238	-239
10	133	-132
11	178	176
12	-20	37
13	116	-127
14	-21	-17
15	84	91
-1	284	299
-2	143	-146
-3	308	-306
-4	-23	-13
-5	234	239
-6	34	-45
-7	224	-241
-8	143	148
-9	190	199
-10	-19	36
-11	176	-173
-12	53	50
-13	148	152
-14	-21	-57
-15	121	-119
-16	-22	31
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1	161	-165
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3	93	89
4	116	-109
5	-19	-4
6	61	46
7	-19	-9
8	87	52
9	53	-9
10	32	-9
11	-21	37
12	-21	24
13	72	-62
-1	132	139
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-3	123	-128
-4	86	82
-5	69	77
-6	-19	39
-7	48	-47
-8	32	-33
-9	33	35
-10	67	-73
-11	-21	-62
-12	-21	15
-13	-21	30
-14	-22	11
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2	133	133
3	120	-111
4	-19	9
5	115	134
6	52	-39
7	144	-146
8	-21	15
9	150	167
10	-22	-40
11	142	-146
-1	126	-127
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-3	170	155
-4	88	-85
-5	134	-143
-6	-20	-24
-7	136	131
-8	-21	23
-9	118	-121
-10	-22	23
-11	133	129
H= 7,K= 8		
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1	32	51
2	70	69
3	33	-45
4	-22	-38
5	36	29
6	37	22
-1	54	-49
-2	82	89
-3	-22	42
-4	32	-34
-5	34	-22
-6	35	27
H= 0,K= 9		
1	179	-81
2	153	-151
3	61	21
4	154	-154
5	58	-55
6	44	15
7	43	28
8	-24	-6
9	-24	-32
10	101	95
11	59	-62
12	111	-102
13	59	36
14	57	-28
15	43	-23
16	41	-51
17	-21	23
18	-22	-10
H= 1,K= 9		
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1	49	-51
2	604	582
3	-21	-0
4	282	-299
5	-22	-25
6	251	241
7	-24	29
8	359	-376
9	103	-103
10	222	226
11	56	80
12	250	-252
13	113	-103
14	211	209
15	33	8
16	116	-105
17	-21	10
18	86	80
-1	70	71
-2	399	376
-3	-21	-30
-4	454	-465
-5	50	-68
-6	228	215
-7	-24	-22
-8	197	-199
-9	49	46
-10	334	330
-11	-21	-44
-12	321	-331
-13	105	106
-14	193	207
-15	32	-24
-16	177	-178
-17	-21	-9
-18	107	99
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1	90	94
2	-22	41
3	101	-92
4	120	-131
5	-24	34
6	166	172
7	-24	-25
8	-23	-23
9	-23	2
10	105	113
11	93	78
12	-19	3
13	32	-47
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15	-21	20
16	-21	-22
17	-21	-29
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-5	-24	-22
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-7	79	85
-8	124	-128
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-10	-22	-3
-11	-20	-4
-12	-19	18
-13	-19	-19
-14	-19	-18
-15	-20	-14
-16	-21	-20
-17	-21	4
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1	123	121
2	304	-286
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4	397	384
5	-23	9
6	303	-296
7	-23	34
8	332	328
9	-20	-16
10	276	-272
11	62	-70
12	143	152
13	53	74
14	99	-109
15	53	-27
16	124	123
-1	75	-81
-2	348	-360
-3	52	66
-4	355	374
-5	-24	44
-6	239	-253
-7	82	-89
-8	290	315
-9	71	69
-10	233	-243
-11	60	-46
-12	194	192
-13	33	26
-14	177	-163
-15	-21	26
-16	109	115
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1	44	-52
2	58	-70
3	49	40
4	39	-27
5	57	-68
6	97	-90
7	78	72
8	-19	6
9	30	34
10	34	-32
11	53	-14
12	67	82
13	-21	25
14	33	-59
15	-21	-17
-1	-23	27
-2	-23	-36
-3	-23	-1
-4	-22	22
-5	-21	-5
-6	159	-155
-7	-19	9
-8	59	54
-9	27	-23
-10	51	-60
-11	33	31
-12	79	75
-13	-21	-15
-14	-22	-12
-15	35	1
H= 5,K= 9		
0	290	-285
1	89	-86
2	181	187
3	47	54
4	163	-171
5	30	10
6	245	248
7	78	-77
8	192	-188
9	32	58
10	132	125
11	31	-44
12	123	-130
13	-22	33
-1	44	71
-2	176	182
-3	45	-48
-4	246	-232
-5	48	-52
-6	243	238
-7	66	62
-8	139	-135
-9	31	-46
-10	79	89
-11	51	-3
-12	121	-125
-13	-22	11
H= 6,K= 9		
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1	79	-68
2	115	119
3	32	29
4	90	-83
5	30	-17
6	-21	4
7	-21	3
8	-21	-25
9	-21	-22
10	88	72
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-2	121	116
-3	31	-44
-4	30	-22
-5	-21	20
-6	-21	-23
-7	-21	3
-8	31	-10
-9	32	-29
-10	-22	37
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1	-21	35
2	124	-117
3	-22	-28
4	99	105
-1	-21	-41
-2	124	-125
-3	35	27
-4	118	118
-5	-22	-12
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1	451	-450
2	50	46
3	398	388
4	96	-46
5	330	-343
6	46	-13
7	300	301
8	-23	-20
9	301	-306
10	-22	-28
11	272	278
12	-19	2
13	202	-202
14	-19	30
15	151	146
16	-21	-18
17	114	-112
H= 1,K=10		
0	105	50
1	66	-62
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9	192	187
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7	165	156
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7	141	-137
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10	134	138
11	107	-117
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7	152	-153
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-5	130	-145
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7	52	50
8	88	-79
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H= 1,K=16		
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6	112	-129
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H= 4,K=16		
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H= 0,K=17		
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-7	58	60
H= 2,K=17		
0	45	52
1	33	15
2	55	-34
3	34	-31
4	-21	-15
5	58	59
6	-22	15
-1	-22	18
-2	-21	1
-3	-22	-8
-4	34	3
-5	-22	-21
-6	-22	13
H= 3,K=17		
0	67	54
1	108	-99
2	38	-40
-1	125	98
-2	58	-77
H= 0,K=18		
0	129	-124
1	48	-16
2	129	104
3	-22	6
4	109	-99
H= 1,K=18		
0	-21	14
1	36	2
2	-22	35
3	-22	-3
-1	-22	-18
-2	-22	-20

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[a] The values of h and k are given above each group with the values of l, $10F_o$, $10F_c$ given in that order. A negative F_o indicates an unobserved reflection.

The weighting scheme used in the least-squares refinement was $\sqrt{w} = 1$ if $F_o \leq 14.0$ and $\sqrt{w} = 14.0/F_o$ if $F_o > 14.0$ where F_o is on the scale given in Table IV.

Discussion

The atomic numbering and the bond distances in the molecule are illustrated in Figure 1 and the bond angles in Figure 2. A view down the ring centers is given in Figure 3 showing the configuration in the solid which corresponds to 1,3′-diacetylferrocene.

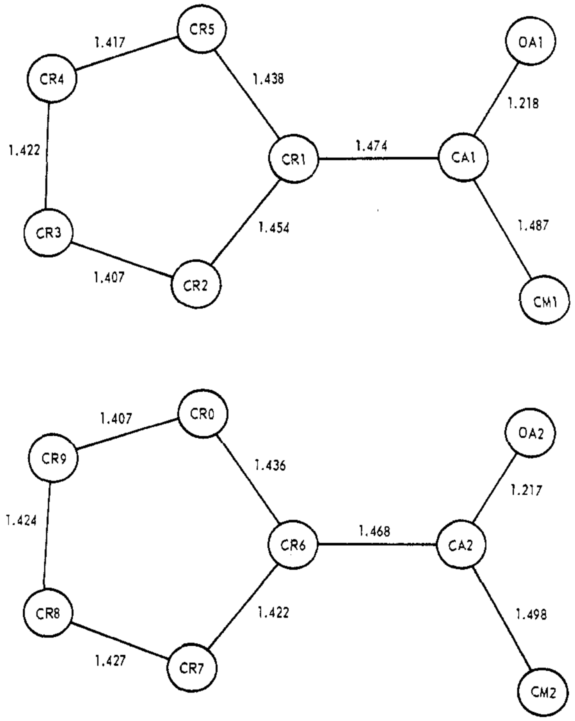

Figure 1.—Atomic numbering and bond distances (in ångströms) in the diacetylferrocene molecule. The estimated standard deviations in bond distances are ±0.007 Å except for C*R*3–C*R*4, C*R*9–C*R*9, C*A*1–C*M*1, and C*A*2–C*M*2 which are ±0.008 Å.

The Cp rings are planar (see Table VI) and nearly parallel, the angle between the planes being 1° 9′. The average C–C distance is 1.428 ± 0.014 Å in ring 1 (atoms C*R*1 to C*R*5) and 1.423 ± 0.014 Å in ring 2 (atoms C*R*6 to C*R*0). The average C–C bond length in both rings is 1.426 ± 0.014 Å, slightly longer than the average value of 1.419 Å cited by Wheatley.[7] However, the average values in more recent structures (bis(π-azulene)iron of 1.430 Å,[3] ferrocenedicarboxylic acid of 1.424 Å,[4] ferrocene (by electron diffraction) of 1.431 Å[8]) are all longer and in excellent agreement. The bond angles in diacetylferrocene average 108.0 ± 0.2°, the value for a regular planar pentagon.

The Fe–C(ring) distances given in Table V vary from 2.030 ± 0.005 to 2.060 ± 0.005 Å, with an average value of 2.046 ± 0.009 Å. The longest Fe–C distances are to C*R*5 and C*R*9 which are opposite each other and to C*R*3 and C*R*8 which are the carbons opposite an acetyl group. The reasons for the slight

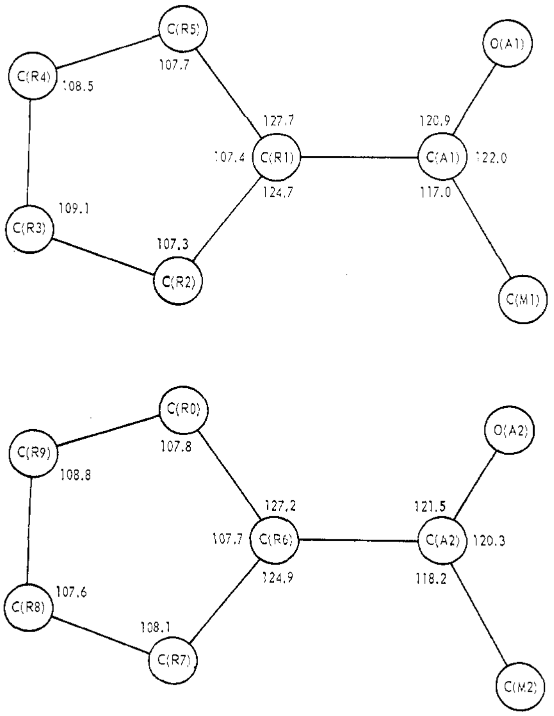

Figure 2.—Bond angles (in degrees) in the diacetylferrocene molecule. The estimated standard deviations in bond angles are ±0.5° except for angles involving C*R*1, C*R*6, C*R*2, C*R*5, C*R*3, and C*R*0 which are ±0.4°.

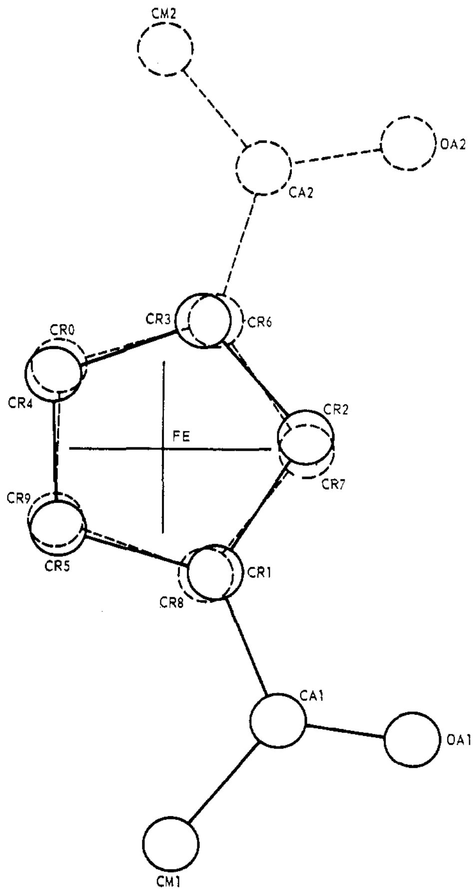

Figure 3.—A view down the ring centers showing the nearly eclipsed configuration of the diacetylferrocene molecule.

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[7] P. J. Wheatley in "Perspectives in Structural Chemistry," Vol. I, J. D. Dunitz and J. A. Ibers, Ed., Wiley, New York, N. Y., 1967, p 9.

shift of the Fe atom are not clear. The average Fe–C (ring) distances agree with those found in bis(π-azulene)-iron of 2.044 Å[3] and in ferrocene of 2.058 Å.[8] The average C–C (cross ring) distance of 3.300 ± 0.014 Å (see Table V) is in agreement with the value of 3.291 Å reported for ferrocenedicarboxylic acid.[4] Therefore, diacetylferrocene has molecular dimensions consistent with other ferrocene molecules and no unusual intramolecular interactions are present.

TABLE V

INTRAMOLECULAR DISTANCES NOT SHOWN IN FIGURE 1

Fe–C*R*1	2.035 (5)	Fe–C*R*8	2.060 (5)
Fe–C*R*2	2.049 (5)	Fe–C*R*7	2.045 (5)
Fe–C*R*3	2.059 (5)	Fe–C*R*6	2.030 (4)
Fe–C*R*4	2.044 (6)	Fe–C*R*0	2.035 (5)
Fe–C*R*5	2.056 (5)	Fe–C*R*9	2.058 (6)
C*R*1–C*R*8	3.313 (7)	Fe–C*A*1	3.076 (5)
C*R*2–C*R*7	3.303 (7)	Fe–O*A*1	3.669 (4)
C*R*3–C*R*6	3.290 (7)	Fe–C*A*2	3.076 (5)
C*R*4–C*R*0	3.271 (7)	Fe–O*A*2	3.832 (4)
C*R*5–C*R*9	3.326 (7)		

The bond lengths in the two acetyl groups are similar to the values expected for C═O, C(sp^2)—C(sp^2), and C(sp^2)—C(sp^3) bond lengths.[9] The variation of the various bond angles from 120° follow a pattern which is determined by nonbonded interactions, similar to the distortions observed in dimethyl *trans,trans*-muconate.[10] The acetyl groups are twisted slightly from (by 11° 1′ for C*A*1–C*M*1–O*A*1 and 8° 48′ for C*A*2–C*M*2–O*A*2) and bent out of the plane of the appropriate Cp ring (see Table VI). However, the two rotations are different so that O*A*1 in one case and C*M*2 in the other are closer to the opposite Cp ring. Presumably this difference in rotation permits better packing in the crystalline state.

A view down the ring centers is given in Figure 3. The angle of twist of the rings was defined as the dihedral angle between a ring carbon, the two ring centers, and the carbon atom on the opposite ring. This angle varied from 4° 15′ to 5° 33′ with an average of 4° 41′. Compared to the configurations of other ferrocene derivatives summarized recently,[3,11] diacetylferrocene is very close to being eclipsed. Since the acetyl groups cannot hydrogen bond and are sufficiently bulky to make disorder in the crystal unlikely, the present configuration must represent the preferred orientation of a disubstituted ferrocene in the absence of a bridge between the two rings. The 1,3′ configuration for diacetylferrocene affords the minimum steric repulsion between acetyl groups which still maintains an eclipsed configuration for the Cp rings. Furthermore, the present study supports the hypothesis that the 1,1′ configuration found in ferrocenedicarboxylic acid was a result of the formation of dimerlike units by hydrogen bonding. Therefore, the concept of the staggered configuration for ferrocenes as the favored geometry is not in agreement with the most recent results. In the absence of steric constraints (and disorder in the crystalline state), the preferred configuration of ferrocene derivatives will be eclipsed or nearly so.

TABLE VI

LEAST-SQUARES PLANES WHERE THE DEVIATIONS FROM THE PLANES (Å) ARE GIVEN FOR THE SPECIFIED ATOM

	Dev from plane			
Atom	I	II	III	IV
C*R*1	0.005	−3.314		
C*R*2	0.002	−3.295		
C*R*3	−0.008	−3.286		
C*R*4	0.011	−3.274		
C*R*5	−0.010	−3.321		
C*A*1	0.118	−3.224	0.000	
C*M*1	−0.100	−3.462	0.000	
O*A*1	0.339	−3.008	0.000	
C*R*6	3.280	0.001		
C*R*7	3.302	0.001		
C*R*8	3.316	−0.004		
C*R*9	3.315	0.005		
C*R*0	3.282	−0.004		
C*A*2	3.171	−0.084	0.000	
C*M*2	2.925	−0.310	0.000	
O*A*2	3.284	0.033	0.000	
Fe	1.650	−1.649		

Parameters for Planes[a]

A	0.2517	0.2513	0.0651	0.1364
B	0.0659	0.0670	0.9934	0.9890
C	0.0602	0.0425	0.0940	−0.0566
D	−0.744	2.488	−0.817	2.003
Atom	I	II	III	IV
Atoms in plane	C*R*1–C*R*5	C*R*6–C*R*0	C*A*1–C*M*1–O*A*1	C*A*2–C*M*2–O*A*2

[a] Equation of plane is of the form $AX + BY + CZ = D$, where X, Y, Z are orthogonal coordinates (in Å) relative to a, b, c^*.

The various ferrocene derivatives reported to date have different angles of rotation of the rings which is not conveyed by the present nomenclature. Therefore, we suggest that the angle of twist of the Cp rings be specified in degrees after the name. The present compound would therefore be called 1,3′-diacetylferrocene (−4.7).

TABLE VII

MEAN-SQUARE DISPLACEMENTS[a]

Atom	$(r^2)^{1/2}$			Atom	$(r^2)^{1/2}$		
C*R*1	201	187	157	C*R*6	211	188	134
C*R*2	225	178	160	C*R*7	214	185	162
C*R*3	238	195	155	C*R*8	243	204	157
C*R*4	242	196	175	C*R*9	234	209	179
C*R*5	210	190	151	C*R*0	218	199	156
C*A*1	210	197	176	C*A*2	217	206	166
C*M*1	317	235	199	C*M*2	261	236	182
O*A*1	284	221	186	O*A*2	280	236	199
Fe	175	164	157				

[a] Values ×10^3 in ångströms.

The thermal parameters were converted to mean-square displacements and are given in Table VII. For the ring atoms, C*R*1–C*R*0, the smallest mean-

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(8) A. Haaland and J. E. Nikson, *Chem. Commun.*, 88 (1968).

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(10) S. E. Filippakio, L. Leiserowitz, and G. M. J. Schmidt, *J. Chem. Soc. B*, 290 (1967).

(11) The value for α-keto-1,1′-trimethyleneferrocene of 11.8° reported by N. D. Jones, R. E. Marsh, and J. H. Richards, *Acta Crystallogr.*, **19**, 330 (1965), and quoted in ref 3 is in error. The correct value is 5.8°: R. E. Marsh, private communication.

TABLE VIII

INTERMOLECULAR DISTANCES[a]

Atom A	Equiv position	Translation	Atom B	Distance A–B, Å
H9	2	0, 0, 1	H11	2.54
H9	2	0, 0, 1	H12	2.44
H9	2	0, 0, 1	H13	2.54
H9	1	1, 0, 0	H7	2.71
H10	1	1, 0, 0	H7	2.50
H11	2	0, 0, 1	H11	2.65
H12	2	1, 0, 1	H8	2.66
H2	1	−1, 0, 0	H4	2.48
H3	2	1, 0, 0	H21	2.78
H4	2	0, 0, 0	H21	2.76
H4	1	1, 0, 0	H7	2.79
C*M*1	2	0, 0, 1	H9	2.75
O*A*1	1	−1, 0, 0	H5	2.58
O*A*1	1	−1, 0, 0	H11	2.88
O*A*1	2	1, 0, 0	H8	2.67
O*A*1	3	1, 1, 1	H22	2.91
C*R*9	1	1, 0, 0	H7	2.99
O*A*2	1	−1, 0, 0	H4	2.96
O*A*2	1	−1, 0, 0	H10	2.72
O*A*2	2	1, 0, 0	H3	2.67
O*A*2	3	1, 0, 1	H13	2.67
C*R*4	1	1, 0, 0	H2	2.99
O*A*1	3	1, 1, 1	C*A*2	3.168
O*A*1	3	1, 1, 1	C*M*2	3.39

[a] The interatomic distance is from A in the equivalent position specified to B in position 1. The code is 1 is x, y, z; 2 is $-x, -y, -z$; 3 is $-x, -\frac{1}{2} + y, -\frac{1}{2} - z$, with the unit translations given with respect to x, y, and z.

square displacement is approximately normal to the plane of the ring, with the largest displacement usually in the plane of the ring. Hence the displacements are in agreement with an oscillation of the rings about the ring centers. In the acetyl groups the largest mean-square displacement is normal to the plane of the acetyl group, in agreement with a wagging motion about the corresponding C–C bond. The fact that the mean-square displacements are in excellent agreement with the expected molecular vibrations suggests that absorption errors are minimal and that the integrated intensity was indeed measured in the data collection process.

All the interatomic distances less than 3.5 Å were calculated and surveyed for any unusual interactions. The H–H contacts less than 2.8 Å together with the H–heavy atom contacts less than 3.0 Å and heavy atom–heavy atom contacts less than 3.4 Å are tabulated in Table VIII. Assuming the usual van der Waals radii,[12] the shortest contacts are simply van der Waals contacts between the appropriate atoms.

Acknowledgments.—The author wishes to thank the National Research Council of Canada and the U. S. Naval Weapons Center for financial support of this research.

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Crystallographic Studies on Sulfur Dioxide Insertion Compounds. I. The Butadieneiron Tricarbonyl–Sulfur Dioxide–Boron Trifluoride Adduct

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The reaction of BF_3 gas with a solution of butadieneiron tricarbonyl in SO_2 has been shown to give rise to a compound of stoichiometry $C_4H_6Fe(CO)_3 \cdot SO_2 \cdot BF_3$. The structure of this species has been elucidated by single-crystal X-ray diffraction studies. The compound crystallizes in the noncentrosymmetric monoclinic space group $P2_1$ (C_2^2; no. 4) with $a = 6.583 \pm 0.011$ Å, $b = 11.782 \pm 0.023$ Å, $c = 7.401 \pm 0.009$ Å, $\beta = 92.41 \pm 0.06°$, $Z = 2$, $\rho_{calcd} = 1.886$ g cm^{-3}, and $\rho_{obsd} = 1.79 \pm 0.05$ g cm^{-3}. Intensity data complete to $\sin \theta = 0.40$ (Mo Kα radiation) were collected on a 0.01°-incrementing Supper-Pace Buerger automated diffractometer, and the structure was solved using Patterson, Fourier, and least-squares refinement techniques; all nonhydrogen atoms were located accurately, the final discrepancy index being $R_F = 6.60\%$ for the 813 independent, nonzero reflections. The inserted sulfur dioxide molecule is S bonded to a terminal methylene group of the modified butadiene ligand (which, now, is involved in a π-allyl$\rightarrow$Fe(CO)$_3$ linkage) and is O bonded to the central iron atom. The remaining oxygen of the SO_2 moiety is linked to the boron atom of a BF_3 molecule.

Introduction

Transition metal complexes containing sulfur dioxide as a ligand are well known;[2] infrared and X-ray diffraction studies[3] have shown that the SO_2 molecule bonds to the metal through its sulfur atom. Wojcicki and coworkers have systematically investigated SO_2 as an insertion ligand and have shown that it inserts into a metal–alkyl or metal–aryl bond (M–R) to produce an *S*-sulfinate[4–10]

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