culations were carried out on the CDC 3200/3600 computers of the CSIRO Division of Computing Research, using programs written or adapted by Dr. J. F. Blount, and on an IBM 360/50 computer at the Computer Centre, Australian National University, with refinement and function-error programs supplied by Dr. W. T. Robinson. The diffraction data were recorded on an automatic diffractometer operated under Grant 65/15552 from the Australian Research Grants Committee.

CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY AND CENTER FOR ADVANCED STUDIES,
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The Crystal and Molecular Structure of the Dicesium Salt of the Di-μ-carbonyl-bis[π-(3)-1,2-dicarbollylcarbonyliron] Anion, Cs$_2$[π-(3)-1,2-B$_9$C$_2$H$_{11}$]$_2$Fe$_2$(CO)$_4$·(CH$_3$)$_2$CO·H$_2$O

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The crystal and molecular structure of the dicesium salt of the di-μ-carbonyl-bis[π-(3)-1,2-dicarbollylcarbonyliron] anion, Cs$_2$[π-(3)-1,2-B$_9$C$_2$H$_{11}$]$_2$Fe$_2$(CO)$_4$, has been determined as its acetone hydrate by single-crystal X-ray diffraction methods. Of the 4639 reflections measured by counter diffractometry, 2500 were included in the refinement. The crystal system is triclinic, space group P$\bar{1}$. Crystal data are: $a = 11.57$ (2), $b = 15.19$ (3), $c = 9.35$ (2) Å, $\alpha = 88°\,48$ (5)$'$, $\beta = 76°\,54$ (5)$'$, $\gamma = 112°\,18$ (5)$'$, $d_m = 1.86$ (1) g cm^{-3}, $Z = 2$, $d_c = 1.87$ (1) g cm^{-3}. Structure determination was by the heavy-atom method and refinement was carried out by the block-diagonal least-squares technique with anisotropic thermal parameters for the cesium and iron atoms. Hydrogen atoms were included in calculated positions but not refined. Final values of R and R_1 are 0.045 and 0.052 (0.080 and 0.068 for all 4639 reflections). The anion consists of two B$_9$C$_2$H$_{11}$Fe(CO)$_2$ fragments joined through a double carbonyl bridged Fe–Fe bond of length 2.591 (5) Å. It has a cisoid, almost totally eclipsed, conformation with a close approach to C$_2$ symmetry. The bridge is asymmetric with Fe–C distances of 1.90, 1.98, 1.90, and 1.99 Å (esd's 0.01 Å) around the bridge. The two Fe–Fe–C planes in the bridge make an angle of 164° about the Fe–Fe axis and are inclined away from the icosahedra. The normals from the basal planes of the cages to the Fe atoms make angles of 140 and 142° with the Fe–Fe axis. These angles are larger than in analogous cyclopentadienyl complexes and are presumably so because of H · · · H repulsions between the cages. The normals from Fe to the basal planes of the cages pass through the center of gravity of the plane in each case and are 1.57 and 1.59 (1) Å. The terminal Fe–C carbonyl distances are 1.69 and 1.70 (1) Å. C–O distances are in the range 1.16–1.18 (2) Å. The mean B–B bond length is 1.787 (5) Å; mean B–C is 1.721 (8) Å. Within the crystal the Cs ions are irregularly coordinated to the oxygen atoms of the solvent molecules. The anions pack so that the icosahedra come into contact across the centers of symmetry along the c axis.

Introduction

Hawthorne and his collaborators have shown that the dicarbollyl anion B$_9$C$_2$H$_{11}^{2-}$ forms stable complexes with a variety of transition metal derivatives.[1,2] X-Ray analysis of some of these compounds has revealed that the dicarbollyl cage may be symmetrically π bonded to the metal atom to form a completed icosahedron.[3-5]

Recently, the tetramethylammonium salt of [B$_9$C$_2$H$_{11}$Fe(CO)$_2$]$_2^{2-}$ was synthesized by Hawthorne and Rühle,[6] who suggested that the anion had a stereochemistry similar to the isoelectronic complex *trans*-[π-C$_5$H$_5$Fe(CO)$_2$]$_2$ which has been structurally characterized by X-ray diffraction methods.[7] This analysis of the crystal structure of the dicesium salt of the same anion, undertaken to establish its solid-state stereochemistry, has shown that in this case the anion adopts a cisoid conformation analogous to that found in the newly isolated and characterized *cis*-[π-C$_5$H$_5$Fe(CO)$_2$]$_2$.[8]

Measurement of Crystal and Intensity Data

Professor M. F. Hawthorne kindly supplied a sample of dicesium di-μ-carbonyl-bis[π-(3)-1,2-dicarbollylcarbonyliron]. The crystals were thin, elongated, dark red platelets from which suitable specimens for X-ray study had to be cut. The crystals have been shown by the X-ray analysis to contain one molecule each of acetone and of water of solvation in the asymmetric unit.

Crystal Data.—For Cs$_2$[B$_9$C$_2$H$_{11}$(CO)$_2$Fe]$_2$·(CH$_3$)$_2$CO·H$_2$O the data are: mol wt 830.4, triclinic, $a = 11.57$ (2), $b = 15.19$ (3), $c = 9.35$ (2) Å, $\alpha = 88°\,48$ (5)$'$, $\beta = 76°\,54$ (5)$'$, $\gamma = 112°\,18$ (5)$'$, $V = 1471$ Å^3, $F(000) = 788$, $\mu = 35.2$ cm^{-1}, λ 0.7107 Å.

The unit cell parameters were derived from 25° pre-

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(1) M. F. Hawthorne, D. C. Young, T. D. Andrews, D. V. Howe, R. L. Pilling, A. D. Pitts, M. Reintjes, L. F. Warren, Jr., and P. A. Wegner, *J. Amer. Chem. Soc.*, **90**, 879 (1968).

(2) M. F. Hawthorne, *Accounts Chem. Res.*, **1**, 281 (1968), and references therein.

(3) A. Zalkin, D. H. Templeton, and T. E. Hopkins, *J. Amer. Chem. Soc.*, **87**, 8988 (1965).

(4) A. Zalkin, T. E. Hopkins, and D. H. Templeton, *Inorg. Chem.*, **5**, 1189 (1966).

(5) A. Zalkin, T. E. Hopkins, and D. H. Templeton, *ibid.*, **6**, 1911 (1967).

(6) M. F. Hawthorne and H. W. Rühle, *ibid.*, **8**, 176 (1969).

(7) O. S. Mills, *Acta Crystallogr.*, **11**, 620 (1958).

(8) R. F. Bryan, P. T. Greene, D. S Field, and M. J. Newlands, *Chem. Commun.*, 1477 (1969)..

cession photographs of the three equatorial zones taken using Zr-filtered Mo Kα radiation at room temperature. The errors in the cell edges are estimated at the 1 part in 600 associated with the precession method. The measured density of the complex is 1.86 g cm^{-3} as determined by flotation in a mixture of ethyl iodide and carbon tetrachloride. That calculated for two formula units of the complex per cell is 1.70 g cm^{-3}. This discrepancy alerted us to the possible presence of solvent of crystallization and the cell was later shown to contain two molecules of acetone and two of water. With $Z = 2$ for the total cell contents the calculated density is 1.87 g cm^{-3}.

The possible triclinic space groups are P1 and P$\bar{1}$. No tests were made for pyro- or piezoelectric effects but the choice of P$\bar{1}$ as the more likely space group with $Z = 2$ is confirmed by the successful outcome of the analysis. No molecular symmetry is implied.

Intensity Data.—Diffraction data were collected from a single-crystal fragment of approximate size 0.04 × 0.2 × 0.2 mm mounted on a eucentric goniometer head so that the reciprocal a^* axis was almost parallel with the fiber axis. In this orientation intensity measurements were made using an SDS Sigma 2 computer-controlled Picker four-circle diffractometer. The measurements were made with Mo K radiation, a Zr–Y balanced filter pair being used to reduce the contribution to the diffracted spectra of wavelengths other than the characteristic Kα. Scintillation counting was employed with pulse height analysis. The counter with receiving apertures 4 mm^2 was placed about 30 cm from the crystal. A takeoff angle of 3° was used on the direct beam. ω scans showed the crystal to be uniform and of a suitable mosaicity. Measurements were made using the θ–2θ scanning technique with a scan rate of 1°/min and symmetrical 1.4° scan ranges being used for all reflections. Background measurements were made for 10 sec at both beginning and end of the scan ranges by the stationary crystal–stationary counter method. True background was assumed to be linear within these limits. Linearity of counter response was established for all count rates observed during the experiment.

A measurement cycle was begun with the Zr filter in place. $I_{\text{Zr}} = C_{\text{pZr}} - 0.5(t_{\text{s}}/t_{\text{b}})(C_{\text{b1}} + C_{\text{b2}})$ and $\sigma(I_{\text{Zr}}) = C_{\text{pZr}} + 0.5(t_{\text{s}}/t_{\text{b}})(C_{\text{b1}} + C_{\text{b2}})$, where C_{p} and C_{b} are the counts accumulated during scan and background measurements occupying times t_{s} and t_{b}, respectively. With $I_{\text{Zr}} < 3\sigma(I_{\text{Zr}})$ the reflection was automatically rejected as insignificant, but, if not, the cycle was repeated with the Y filter in place. The net intensity, I, is then given by $C_{\text{pZr}} - C_{\text{pY}} - 0.5(t_{\text{s}}/t_{\text{b}})(C_{\text{b1}} + C_{\text{b2}} - C_{\text{b3}} - C_{\text{b4}})$ and $\sigma^2(I) = C_{\text{pZr}} + C_{\text{pY}} + 0.5(t_{\text{s}}/t_{\text{b}})(C_{\text{b1}} + C_{\text{b2}} + C_{\text{b3}} + C_{\text{b4}})$. Reflections were taken as significant when $I > 3\sigma(I)$.

The reciprocal lattice was examined at 6905 independent lattice points ($2\theta < 60°$) of which 4639 showed significant diffracted intensity. The overall stability of the system was checked by monitoring the intensities of two moderately strong reflections after every 66 measurement cycles. These showed a uniform decrease in intensity of about 10% over the month spent in collecting the diffraction data indicating a gradual breakdown of the lattice structure. An appropriate correction was made for this effect and a single scale factor was used throughout the analysis.

No absorption corrections were made. With $\mu = 35$ cm^{-1} for the crystal used maximum and minimum transmission factors of about 0.9 and 0.5 are to be expected. Such extreme variations were not in fact observed in the intensities of the $h00$ reflections as a function of ϕ where such effects ought to have been most marked. However, there is no doubt that the main residual error in the experimental data is attributable to this cause though much of it may have been apparently compensated by the use of anisotropic thermal parameters for the cesium and iron atoms.

Solution and Refinement of the Structure

Coordinates for the two cesium and two iron atoms in the asymmetric unit were derived from an unsharpened three-dimensional Patterson synthesis calculated with the 1944 largest squared structure amplitudes. For the remaining calculations the 2499 reflections with $|F_{\text{o}}| > 26$ on an absolute scale were used. This gave an adequate yet manageable data set for the Sigma 2 computer used. At the end of the refinement the ratio of observations to parameters was about 14:1.

From these coordinates a structure factor calculation assuming $B = 2.5$ Å^2 gave a conventional R defined as $\Sigma||F_{\text{o}}| - |F_{\text{c}}||/\Sigma|F_{\text{o}}|$ of 0.24. The remaining nonhydrogen atoms of the anion were located by application of the heavy-atom method of phase determination in successive three-dimensional electron density syntheses. At this time all the atoms of the dicarbollide cages were treated as boron. Refinement using the block-diagonal least-squares method and individual isotropic thermal parameters gave $R = 0.11$.

The function minimized was $\Sigma w(|F_{\text{o}}| - |F_{\text{c}}|)^2$. Individual 3 × 3 matrices were used for the positional parameters, 1 × 1 for the isotropic thermal parameters, and 2 × 2 for the overall thermal parameter and scale factor. Unit weights were assigned initially, and in the later stages a scheme which gave $w = I/1500$ for reflections where the observed net peak intensity I was less than 1500 counts, $w = 90/|F_{\text{o}}|$ for structure amplitudes greater than 90 on an observational scale (95 on an absolute scale), and unity to the remainder was used. To ensure smooth convergence the calculated shifts in the light-atom parameters had damping factors of 0.2 applied; the heavy atoms, 0.5.

The remaining atoms of the solvent molecules were located at this point from a three-dimensional difference electron density synthesis using calculated structure factors based on the results of the least-squares refinement thus far.

Seven further cycles of refinement in which all parameters were varied led to convergence with $R = 0.083$. Examination of the agreement between individual observed and calculated structure amplitudes showed that

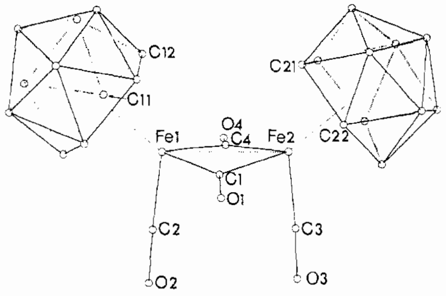

Figure 1.—A general view of the anion showing the numbering scheme adopted for the atoms in the central region and the relative positions of the carbon atoms in the icosahedra.

(020) and (201) had large negative discrepancies presumably caused by extinction. These were given zero weight and five further cycles of refinement led to $R = 0.079$.

It was now possible to identify unambiguously the carbon atoms in the dicarbollide cages by the following criteria: (1) two adjacent atoms in each cage in the five-membered ring bonded to iron had much lower thermal parameters than their neighbors; (2) a ($\rho_o - \rho_c$) synthesis evaluated in the plane of the ring on the assumption of equal boron atoms showed regions of positive density at these same atomic sites in each case; (3) the interatomic separation between these pairs of atoms in each case was closer to that expected for a C–C bond than for B–B or B–C.[3] These atoms were therefore assumed to be carbon and four further cycles of refinement gave convergence with $R = 0.077$.

A further three-dimensional ($\rho_o - \rho_c$) synthesis showed evidence of thermal anisotropy in the vibrations of the cesium and iron atoms. With our available computing facilities it would have been impracticable to refine anisotropic thermal parameters for all atoms; indeed with the uncorrected absorption effects it would probably not have produced physically significant results. However, anisotropic thermal parameters were assigned to the four metal atoms and refined using 6 × 6 blocks in a further six cycles to convergence at $R = 0.048$. The contributions of the light atoms to the structure factors were held fixed during this process at their previous values. R_1 defined as $[\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2]^{1/2}$ was 0.057 and the standard deviation of an observation of unit weight was 3.2.

From the geometry of the complex it seemed clear that some knowledge of the hydrogen positions would be helpful in deciding certain questions and so an attempt was made to locate these atoms. No great success was anticipated since the fraction of the total scattering power of the crystal which they represent is very small indeed. A final three-dimensional ($\rho_o - \rho_c$) synthesis was calculated, however, to check the validity of the proposed solution. This showed that the thermal motion of the metal atoms had been effectively compensated. The largest regions of residual electron density were associated with the two cesium atoms. Each was surrounded by four peaks in a plane of height 0.7–1.0 e$^-$/Å^3 with negative peaks of −1.4 e$^-$/Å^3 in a line perpendicular to the plane. The patterns were identical for both atoms. Of the 19 remaining peaks of density in excess of 0.5 e$^-$/Å^3 (none greater than 0.8 e$^-$/Å^3) 15 occurred at positions which could reasonably be assigned to hydrogen atoms and 4 in positions suggesting thermal anisotropy of the oxygen atoms of the terminal carbonyl groups. The remainder of the function showed random fluctuations less than ±0.4 e$^-$/Å^3.

Calculated positions for the hydrogen atoms were derived on the assumption of icosahedral geometry for the $B_9C_2H_{11}$ fragment, the hydrogen centers being located on the extensions of the pseudo-fivefold axis with B–H = 1.20 and C–H 1.10 ± 0.01 Å. The mean deviation between these calculated positions and those observed is 0.29 Å.

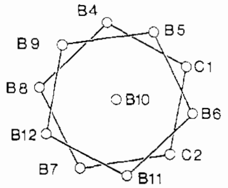

Figure 2.—Diagrammatic representation of the numbering scheme adopted for the atoms of the icosahedral fragment. The iron atom is assumed to occupy the 3 position. In the tables and text the prefixes 1 or 2 are added before the number of the atom to distinguish the atoms of one cage from those of the other.

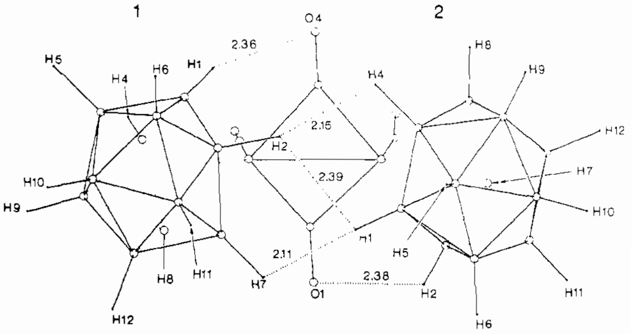

Figure 3.—A general view of the anion showing the *calculated* positions for the hydrogen atoms and the shorter intramolecular approach distances resulting. Since the model for the hydrogens may be imperfect (see text), this illustration should be taken only as a guide to which atoms are in contact in the actual structure.

A structure factor calculation for the 2499 reflections used in the refinement which included the contributions of the hydrogen atoms in their calculated positions with isotropic B values of 3.0 Å^2 reduced R to 0.045, R_1 to 0.052, and the standard deviation of an observation of unit weight to 2.95. We may therefore be reasonably confident that their inclusion is justified. A final structure factor calculation over all 4639 significant reflections gave $R = 0.080$, $R_1 = 0.068$. All calculations described were carried out using programs written in this laboratory for the 16K SDS Sigma 2 computer.

The scattering functions used for the neutral atoms were taken from Hanson, *et al.*;[9] that for Cs$^+$ was taken

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[9] H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Crystallogr.*, **17**, 1040 (1964).

TABLE I

Final Positional and Thermal Parameters[a]

Atom	x	y	z	B, Å	Atom	x	y	z	B, Å
Cs_1	−5300 (1)	1833 (1)	3943 (1)		B_{25}	2272 (14)	778 (11)	53 (17)	2.1 (3)
Cs_2	−2557 (1)	3217 (1)	−641 (1)		B_{26}	1691 (17)	1150 (13)	−1353 (20)	3.2 (3)
Fe_1	258 (2)	2718 (1)	3403 (2)		B_{27}	3243 (14)	3117 (11)	−1184 (17)	2.1 (3)
Fe_2	2054 (2)	2881 (1)	1055 (2)		B_{28}	3914 (13)	2757 (10)	255 (16)	1.7 (2)
O_1	−283 (10)	3046 (7)	599 (11)	3.5 (2)	B_{29}	3886 (16)	1594 (12)	−164 (18)	2.6 (3)
O_2	876 (12)	4739 (9)	3384 (13)	5.0 (3)	B_{210}	3320 (16)	1261 (12)	−1778 (19)	2.9 (3)
O_3	3252 (12)	4931 (9)	725 (14)	5.2 (3)	B_{211}	2894 (18)	2180 (14)	−2339 (21)	3.5 (4)
O_4	2821 (9)	3070 (7)	3820 (11)	3.1 (2)	B_{212}	4266 (16)	2502 (13)	−1641 (19)	2.9 (3)
O_5	−3277 (12)	3861 (9)	2494 (14)	5.3 (3)	H_{11}	93	237	576	3.0
O_6	−3417 (13)	1255 (10)	1235 (16)	6.4 (3)	H_{14}	−66	348	581	
C_1	319 (12)	2923 (9)	1372 (14)	2.2 (2)	H_{112}	−383	60	452	
C_2	629 (14)	3907 (10)	3428 (16)	2.9 (3)	H_{111}	−203	−44	453	
C_3	2758 (14)	4100 (11)	859 (17)	3.2 (3)	H_{12}	57	112	367	
C_4	2113 (11)	2961 (8)	3058 (13)	1.6 (2)	H_{15}	−140	183	824	
C_5	−2836 (17)	4514 (13)	3155 (20)	4.8 (4)	H_{19}	−346	199	680	
C_6	−1584 (27)	5364 (20)	2578 (31)	9.3 (7)	H_{17}	−130	124	210	
C_7	−3640 (32)	4572 (24)	4655 (37)	11.6 (9)	H_{18}	−216	274	350	
C_{11}	−8 (12)	2022 (9)	5532 (13)	1.8 (2)	H_{110}	−337	3	737	
C_{12}	−209 (12)	1301 (9)	4283 (14)	2.1 (2)	H_{16}	−55	32	682	
B_{14}	−939 (15)	2679 (11)	5535 (17)	2.2 (3)	H_{21}	44	109	115	
B_{15}	−1385 (15)	1695 (11)	6966 (18)	2.4 (3)	H_{22}	103	249	−117	
B_{16}	−889 (16)	811 (12)	6150 (18)	2.6 (3)	H_{24}	256	153	252	
B_{17}	−1330 (14)	1348 (11)	3384 (16)	1.9 (3)	H_{25}	193	−5	49	
B_{18}	−1829 (15)	2250 (11)	4179 (17)	2.2 (3)	H_{26}	93	60	−192	
B_{19}	−2576 (15)	1812 (11)	6118 (17)	2.4 (3)	H_{27}	359	394	−161	
B_{110}	−2532 (13)	646 (10)	6461 (15)	1.5 (2)	H_{28}	469	332	81	
B_{111}	−1742 (14)	369 (10)	4784 (16)	1.7 (2)	H_{29}	468	134	12	
B_{112}	−2815 (14)	978 (11)	4796 (17)	2.1 (3)	H_{210}	370	78	−259	
C_{21}	1401 (13)	1452 (10)	455 (15)	2.5 (3)	H_{211}	297	236	−363	
C_{22}	1748 (12)	2269 (9)	−920 (15)	2.4 (3)	H_{212}	533	289	−243	
B_{24}	2654 (14)	1698 (11)	1220 (17)	2.1 (3)					

Anisotropic Thermal Parameters[b]

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}		β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cs_1	575 (9)	486 (6)	1777 (14)	146 (6)	−65 (9)	27 (7)	Fe_1	375 (16)	249 (10)	594 (23)	137 (10)	−42 (15)	−18 (12
Cs_2	723 (10)	548 (6)	1113 (14)	336 (6)	−144 (9)	−179 (7)	Fe_2	357 (16)	255 (10)	575 (24)	115 (10)	−29 (15)	34 (12

[a] The positional parameters are expressed as fractions of the respective cell edges $\times 10^4$ ($\times 10^3$ in the case of the hydrogen atoms). Standard deviations are given in parentheses and attach to the last significant figure. These esd's are obtained according to the formula $\sigma^2(x) = a^{ij}\Sigma w\Delta^2/(n - m)$ where a^{ij} is obtained by inversion of the appropriate matrix (a_{ij}), w is the weight assigned an observational discrepancy $\Delta = F_o - F_c$, n is the number of observations, and m is the number of variable parameters. In calculating the contribution to the structure factors of the hydrogen atoms a value of $B = 3.0$ Å^2 was taken in the exponent for the thermal parameter in each case. [b] Anisotropic thermal parameters are $\times 10^5$ with esd's in parentheses on the same scale. The thermal parameter T has the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

from Cromer and Waber.[10] The curves for both Cs and Fe were corrected for the real part of the anomalous dispersion effect by −0.53 and 0.37 e$^-$, respectively.[11]

Results and Discussion

The atomic parameters defining the crystal structure, together with their estimated standard deviations (esd's), are given in Table I. Table II provides a comparison between the observed structure amplitudes and structure factors calculated from the parameters of Table I. Interatomic distances and angles, with their associated esd's, calculated from the same parameters are given in Table III.

Figure 1 shows a general view of the structure of the anion and illustrates the numbering scheme adopted for the atoms in the central region. In labeling the atoms of the icosahedra the convention has been adopted that the iron atom occupies the 3 position and the other atoms are numbered as shown in Figure 2. The prefix 1 or 2 is added to distinguish the atoms of one cage from those of the other.

Table IV lists the equations of the least-squares planes through certain atomic groupings of interest while Table V gives the shorter intra- and intermolecular approach distances. The most critical intramolecular interactions are also shown in Figure 3 which illustrates the *calculated* positions of the hydrogen atoms. A view of the packing of the ions and solvent molecules in the crystal is shown in Figure 4.

The crystal structure, as expected, is ionic. Our interest is primarily in the structure of the anion. The two iron-containing icosahedra are joined through a doubly carbonyl-bridged Fe–Fe bond. Each iron atom may be assumed to reach an inert gas configuration by accepting five electrons from the carborane fragment, two from the terminal, one each from the bridging carbonyl groups, and one by formation of an Fe–Fe bond.

This bond is slightly longer than any other known

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(10) D. T. Cromer and J. T. Waber, *Acta Crystallogr.*, **18**, 104 (1965).

(11) D. T. Cromer, *ibid.*, **18**, 17 (1965).

TABLE II

LIST OF OBSERVED STRUCTURE AMPLITUDES AND CALCULATED STRUCTURE FACTORS[a]

***** H = 0 *****			
0	1	291	307
0	2	1226	1127
0	3	1191	1132
0	4	1590	-1514
0	6	626	-590
0	7	479	-504
1	8	293	304
1	7	797	792
1	5	1512	1506
1	3	941	-894
1	2	1841	1682
1	1	1826	-2015
1	-1	314	310
1	-2	1424	-1325
1	-3	468	392
1	-4	358	-391
1	-5	265	-285
1	-10	318	339
2	-6	837	896
2	-5	518	496
2	-4	1046	1007
2	-3	488	484
2	-2	555	-549
2	-1	442	-443
2	1	389	-320
2	2	646	-618
2	3	1597	-1516
2	4	1158	1086
2	5	551	-499
2	7	385	329
3	8	338	-360
3	7	716	-731
3	5	1631	-1556
3	4	445	403
3	1	1789	2029
3	-1	1271	1246
3	-2	812	752
3	-3	302	-298
3	-5	334	-355
3	-7	278	-236
3	-10	267	-307
4	-9	364	376
4	-8	280	-319
4	-6	508	-511
4	-5	629	-605
4	-4	315	-284
4	-3	812	-825
4	-2	267	227
4	-1	645	-994
4	0	278	293
4	2	492	-484
4	3	1154	1179
4	6	859	869
4	8	340	340
5	8	508	519
5	5	771	812
5	4	640	-650
5	3	323	-328
5	2	861	-893
5	1	1451	-1612
5	0	1040	-1060
5	-1	1272	-1240
5	-4	843	840
5	-5	883	921
5	-7	578	612
6	-9	375	-418
6	-5	535	541
6	-4	691	-695
6	-2	483	449
6	0	929	951
6	1	769	696
6	2	764	796
6	3	420	410
6	6	969	-1001
6	8	519	-532
6	9	350	-378
6	10	281	265
7	11	275	-269
7	8	308	-295
7	7	364	379
7	4	496	481
7	2	649	680
7	1	369	365
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0	-1	616	-594
0	1	613	-685
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2	6	691	-735
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4	-1	607	601
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4	2	516	-502
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5	3	608	658
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5	-3	596	-596
6	-4	515	-548
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7	1	793	-759
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8	-2	298	-319
8	-1	515	469
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8	6	327	-326
8	9	333	-328
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9	0	343	-298
9	-3	392	-409
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7	-6	278	293
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7	2	291	-306
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6	8	270	-246
6	7	279	274
6	5	285	-266
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-4	-5	410	427
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-5	-3	333	329
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-9	-7	440	-441
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TABLE II (*Continued*)

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3	4	330	-359
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-7	-4	281	-278
-7	-3	633	-580
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7	4	477	-469
7	0	279	268
8	2	265	231
9	4	355	318
****** H = 11 *****			
5	6	349	-359
4	5	361	384
4	1	368	-347
3	0	301	249
3	3	328	334
3	6	305	339
2	5	646	-696
2	1	482	509
1	0	638	-630
1	3	435	-476
1	4	424	430
1	7	338	330
0	5	455	475
0	2	443	468
0	1	396	-447
-1	-3	322	312
-1	-2	295	272
-1	0	789	801
-1	4	630	-652
-1	7	344	-323
-2	3	336	341
-2	2	488	-536
-2	0	289	-252
-2	-1	720	-713
-2	-5	299	346
-3	-3	336	-395
-3	0	499	-540
-3	1	333	320
-3	4	488	506
-3	6	267	271
-4	5	394	-385
-4	3	358	-362
-4	-1	797	791
-4	-3	371	387
-4	-4	290	295
-4	-5	367	-386
-5	-6	328	362
-5	-2	396	-368
-5	3	283	-274
-5	5	322	-276
-5	9	347	363
-6	7	324	298
-6	5	634	643
-6	4	513	511
-6	3	298	311
-6	2	349	384
-6	-1	496	-493
-6	-4	417	-369
-7	-2	626	602
-7	0	394	369
-7	4	414	-427
-8	5	310	-288
-8	4	453	-420
-8	2	453	-409
-9	-5	278	-238
-9	-3	280	-319
-9	0	343	-324
-9	1	420	412
-9	3	384	358
-9	4	621	627
-9	6	362	294
-10	3	350	-342
-10	-1	510	470
-11	-1	272	241
-11	1	559	-539
-11	3	560	-549
-11	4	480	-462
-12	3	492	480
-12	2	306	249
-12	-1	467	-450
-12	-2	389	-385
-12	-4	567	-552
-13	-2	361	345
-13	-1	277	-242
-13	1	342	357
-13	3	410	413
-14	3	424	-379
-14	2	489	-475
-14	0	357	-359
-14	-2	267	258
-14	-4	427	428
-15	-2	372	-351
-17	-3	287	239
****** H = 12 *****			
-17	0	370	-354
-15	4	281	-274
-15	0	385	344
-14	-1	282	-279
-14	0	320	-308
-14	1	371	-362
-14	5	442	416
-12	-1	437	402
-12	0	357	312
-12	1	322	355
-12	5	302	-299
-11	8	269	226
-11	6	357	363
-11	5	304	261
-11	0	436	-448
-10	-5	397	417
-10	-4	297	311
-10	-2	470	447
-10	2	388	-404
-9	3	556	530
-9	1	450	424
-9	0	705	665
-9	-4	350	-368
-8	-4	265	-249
-8	-2	483	-474
-8	1	399	-392
-7	7	360	337
-7	3	688	-697
-7	1	394	-393
-7	0	683	-631
-7	-4	431	454
-6	1	879	852
-6	4	513	479
-6	5	399	-406
-6	8	330	-352
-5	6	382	355
-5	3	404	409
-5	2	266	-277
-5	-1	304	-300
-5	-3	305	-309
-4	-3	277	236
-4	1	735	-713
-4	2	280	-278
-4	4	536	-566
-4	5	323	327
-4	8	292	299
-3	9	281	-261
-3	6	448	-481
-3	2	450	461
-2	-4	377	-399
-2	-2	449	-451
-2	2	275	265
-2	4	365	359
-1	9	277	275
-1	4	264	-243
-1	3	448	-482
-1	2	392	-395
-1	-1	283	263
1	3	494	514
1	1	346	334
1	-1	418	-418
1	-3	466	-470
2	-1	280	-260
2	0	332	303
2	4	311	-316
3	1	336	-326
4	2	406	410
4	4	386	437
5	5	269	-306

[a] The columns contain, in sequence: $k, l, 10|F_o|, 10F_c$.

TABLE III

INTERATOMIC DISTANCES AND ANGLES[a]

Bond Lengths

Fe_1–Fe_2	2.591 (5)		
Fe_1–C_1	1.900 (14)	Fe_2–C_4	1.895 (13)
Fe_1–C_2	1.692 (15)	Fe_2–C_3	1.703 (13)
Fe_1–C_4	1.981 (12)	Fe_2–C_1	1.987 (13)
C_1–O_1	1.17 (2)	C_4–O_4	1.17 (2)
C_3–O_3	1.16 (2)	C_2–O_2	1.18 (2)
Fe_1–C_{11}	2.136 (13)	Fe_2–C_{21}	2.144 (14)
Fe_1–C_{12}	2.108 (13)	Fe_2–C_{22}	2.126 (14)
Fe_1–B_{14}	2.139 (16)	Fe_2–B_{24}	2.171 (16)
Fe_1–B_{17}	2.197 (15)	Fe_2–B_{27}	2.166 (16)
Fe_1–B_{18}	2.178 (16)	Fe_2–B_{28}	2.193 (14)
Fe_1–cg_1	1.572 (10)	Fe_2–cg_2	1.586 (10)

Dicarbollide Cages[b]

C_1–C_2	1.61 (2)	1.64 (2)	B_4–B_9	1.80 (2)	1.75 (2)
C_1–B_4	1.72 (2)	1.68 (2)	B_4–B_5	1.82 (2)	1.78 (2)
C_1–B_6	1.74 (2)	1.75 (2)	B_6–B_{11}	1.78 (2)	1.72 (3)
C_1–B_5	1.73 (2)	1.68 (2)	B_5–B_6	1.77 (2)	1.78 (2)
C_2–B_7	1.72 (2)	1.68 (2)	B_6–B_{10}	1.77 (2)	1.78 (2)
C_2–B_6	1.76 (2)	1.74 (2)	B_{11}–B_{12}	1.81 (2)	1.76 (2)
C_2–B_{11}	1.75 (2)	1.70 (2)	B_{10}–B_{11}	1.77 (2)	1.75 (3)
B_7–B_8	1.79 (2)	1.87 (2)	B_9–B_{12}	1.78 (2)	1.79 (3)
B_7–B_{11}	1.80 (2)	1.78 (2)	B_{10}–B_{12}	1.76 (2)	1.81 (3)
B_7–B_{12}	1.79 (2)	1.76 (2)	B_5–B_9	1.80 (2)	1.77 (2)
B_4–B_8	1.79 (2)	1.76 (2)	B_9–B_{10}	1.82 (2)	1.79 (2)
B_8–B_{12}	1.83 (2)	1.81 (2)	B_5–B_{10}	1.80 (2)	1.81 (2)
B_8–B_9	1.81 (2)	1.81 (2)			

Acetone Molecule

C_5–C_6	1.50 (3)	C_5–C_7	1.52 (4)
C_5–O_5	1.19 (2)		

Bond Angles

Fe_1–Fe_2–C_1	46.7 (4)	Fe_2–Fe_1–C_4	46.6 (4)
Fe_1–Fe_2–C_3	95.7 (5)	Fe_2–Fe_1–C_2	96.0 (5)
Fe_1–Fe_2–C_4	49.5 (4)	Fe_2–Fe_1–C_1	49.6 (4)
Fe_1–C_1–Fe_2	83.6 (5)	Fe_1–C_4–Fe_2	83.9 (5)
Fe_1–C_1–O_1	142 (1)	Fe_2–C_4–O_4	141 (1)
Fe_1–C_2–O_2	177 (1)	Fe_2–C_3–O_3	179 (2)
Fe_1–C_4–O_4	135 (1)	Fe_2–C_1–O_1	135 (1)
C_1–Fe_1–C_2	86.5 (6)	C_3–Fe_2–C_4	85.3 (6)
C_1–Fe_1–C_4	95.1 (5)	C_1–Fe_2–C_4	95.0 (5)
C_2–Fe_1–C_4	89.7 (6)	C_1–Fe_2–C_3	90.5 (5)

Acetone Molecule

O_5–C_5–C_6	126 (2)	O_5–C_5–C_7	119 (2)
C_6–C_5–C_7	115 (2)		

Icosahedra[b]

Fe–C_1–C_2	66.8 (6)	66.9 (7)	Fe–B_4–C_1	66.2 (7)	66.2 (7)
Fe–C_1–B_4	66.3 (7)	68.0 (7)	Fe–B_4–B_8	66.6 (7)	66.9 (7)
Fe–C_2–C_1	68.6 (6)	68.0 (7)	C_1–Fe–C_2	44.6 (5)	45.1 (5)
Fe–C_2–B_7	69.2 (7)	68.3 (7)	C_2–Fe–B_7	47.0 (5)	46.0 (5)
Fe–B_7–C_2	63.8 (6)	65.7 (7)	B_7–Fe–B_8	48.3 (6)	50.7 (6)
Fe–B_7–B_8	65.3 (7)	65.4 (7)	C_1–Fe–B_4	47.6 (5)	45.8 (5)
Fe–B_8–B_7	66.4 (7)	63.9 (6)	B_4–Fe–B_8	49.0 (6)	47.5 (6)
Fe–B_8–B_4	64.3 (7)	65.6 (7)	Fe–Fe–cg	139.8 (2)	141.8 (2)
C_1–C_2–B_6	61.9 (8)	62.5 (9)	C_1–B_4–B_5	58.3 (8)	58.2 (8)
C_1–B_6–C_2	54.9 (8)	55.9 (8)	C_1–B_6–B_5	59.0 (9)	56.9 (9)
C_1–B_5–B_4	58.1 (8)	58.1 (8)	C_1–B_5–B_6	59.6 (9)	60.8 (9)
C_2–C_1–B_6	63.3 (8)	61.5 (9)	C_2–B_7–B_{11}	59.5 (8)	58.7 (9)
C_2–B_6–B_{11}	59.2 (8)	58.9 (10)	C_2–B_{11}–B_7	57.9 (8)	57.6 (9)
C_2–B_{11}–B_6	59.9 (8)	61.2 (10)	B_7–B_2–B_{11}	62.6 (8)	63.8 (9)
B_7–B_8–B_{12}	59.4 (8)	57.0 (8)	B_7–B_{11}–B_{12}	59.6 (8)	59.5 (10)
B_7–B_{12}–B_8	59.2 (8)	63.1 (9)	B_7–B_{12}–B_{11}	60.1 (8)	61.1 (10)
B_8–B_7–B_{12}	61.4 (9)	59.9 (9)	B_8–B_4–B_9	60.6 (9)	61.9 (9)
B_8–B_{12}–B_9	60.2 (9)	60.3 (9)	B_8–B_9–B_4	59.6 (9)	59.1 (8)
B_8–B_9–B_{12}	61.3 (9)	60.5 (9)	B_4–B_1–B_5	63.7 (9)	63.7 (9)
B_4–B_8–B_9	59.8 (9)	58.9 (9)	B_4–B_9–B_5	60.8 (9)	60.5 (9)
B_4–B_5–B_9	59.5 (9)	59.3 (9)	B_6–C_1–B_5	61.5 (9)	62.3 (9)
B_6–C_2–B_{11}	60.9 (8)	59.9 (10)	B_6–B_{11}–B_{10}	60.0 (8)	61.6 (10)
B_6–B_5–B_{10}	59.6 (9)	59.3 (9)	B_6–B_{10}–B_{11}	60.2 (8)	58.2 (10)
B_6–B_{10}–B_5	59.4 (9)	59.5 (9)	B_{11}–B_7–B_{12}	60.3 (8)	59.5 (10)
B_{11}–B_6–B_{10}	59.8 (8)	60.3 (10)	B_{11}–B_{12}–B_{10}	59.5 (8)	58.9 (10)
B_{11}–B_{10}–B_{12}	61.4 (8)	59.0 (10)	B_9–B_8–B_{12}	58.5 (9)	59.2 (9)
B_{12}–B_{11}–B_{10}	59.1 (8)	62.1 (10)	B_{12}–B_9–B_{10}	58.8 (8)	60.9 (10)
B_9–B_{10}–B_{12}	59.5 (8)	59.5 (10)	B_9–B_4–B_5	59.6 (9)	60.1 (9)
B_9–B_{12}–B_{10}	61.7 (9)	59.6 (10)	B_9–B_5–B_{10}	60.6 (8)	59.9 (9)
B_9–B_{10}–B_5	59.7 (8)	58.9 (9)	B_5–B_6–B_{10}	61.0 (9)	61.2 (9)
B_5–B_9–B_{10}	59.7 (8)	61.2 (9)			

[a] Distances are in ångströms and angles in degrees. Esd's are given in parentheses and affect the least significant figure. In calculating the esd's, no account has been taken of possible correlations between the parameters of different atoms but account has been taken of correlations between the parameters of an individual atom due to the nonorthogonality of the cell axes and of the effect of possible errors in the cell constants at the level quoted. cg denotes the center of gravity of the five-membered ring bonded to iron. [b] The numbering scheme for the dicarbollide cages is that given in Figure 3. The first column gives distances or angles in the icosahedron of which Fe_1 is a part; the second column, the corresponding parameter for the Fe_2 icosahedron.

doubly carbonyl-bridged Fe–Fe linkage. Its length may be compared with the value of 2.508 (3) Å found[12a] in diazulenetetrairon decacarbonyl, the 2.534 (2) Å observed[12b] in *trans*-$[\pi\text{-}C_5H_5Fe(CO)_2]_2$, the 2.533(6) Å noted[8] in the *cis* isomer of the same complex, and the 2.558 (9) and 2.568 (8) Å established[13] for the two isomers of $Fe_3(CO)_{11}P(C_6H_5)_3$.

As in the last named complex, the carbonyl bridges

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(12) (a) M. R. Churchill and P. H. Bird, *Inorg. Chem.*, **8**, 1941 (1969); (b) R. F. Bryan and P. T. Greene, *J. Chem. Soc. A*, in press.

(13) D. J. Dahm and R. A. Jacobson, *J. Amer. Chem. Soc.*, **90**, 5106 (1968).

TABLE IV

SELECTED LEAST-SQUARES PLANES

Equations of Planes in the Form $AX + BY + CZ = D^a$

Atoms	A	B	C	D	Plane
O_5, C_5, C_6, C_7	0.7965	−0.4309	0.4242	−5.8530	1
C_{11}, C_{12}, B_{17}, B_{18}, B_{14}	−0.3714	−0.6217	0.6896	1.2936	2
C_{21}, C_{22}, B_{27}, B_{28}, B_{24}	−0.4733	0.6143	0.6313	1.1277	3
Fe_1, Fe_2, C_1, O_1	0.0577	0.9979	0.0284	4.2336	4
Fe_1, Fe_2, C_4, O_4	0.1681	−0.9773	0.1294	−3.7884	5

Distances of Atoms from Planes, Å[b]

Atom	1	Atom	2	3	Atom	4	5
O_5	0.013	C_1	−0.019	0.002	Fe_1	−0.003	−0.002
C_5	−0.033	C_2	0.016	0.000	Fe_2	−0.002	−0.002
C_6	0.010	B_7	−0.006	−0.002	C	0.011	0.009
C_7	0.009	B_8	−0.005	0.003	O	−0.006	−0.005
		B_4	0.014	−0.003			

[a] X, Y, Z are in ångströms; the transformation matrix relating the triclinic coordinates to these Cartesian coordinates is

$$\begin{array}{ccc} 11.5700 & -5.7601 & 2.1260 \\ 0.0 & 14.0544 & 1.0755 \\ 0.0 & 0.0 & 9.0424 \end{array}$$

All atoms were given equal weight in calculating these planes. [b] See footnote *b* to Table III.

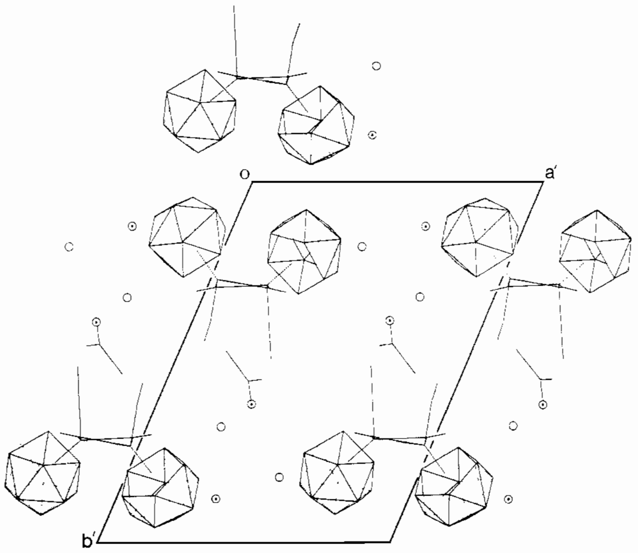

Figure 4.—A view of the crystal structure in projection down the crystallographic *c* axis showing the packing of ions and solvent molecules. Oxygen atoms in the solvent molecules are denoted by the circles with dots; Cs^+ ions, by the open circles.

TABLE V

SELECTED INTRA- AND INTERMOLECULAR CONTACTS

(a) Intramolecular Contacts Less Than 3.40 Å Not Involving Hydrogen

Atoms	Dist, Å	Atoms	Dist, Å
$C_2\cdots B_{14}$	2.51	$O_4\cdots C_{11}$	3.06
$C_3\cdots B_{27}$	2.54	$O_1\cdots C_{22}$	3.10
$C_4\cdots B_{24}$	2.75	$C_2\cdots C_{11}$	3.18
$C_1\cdots B_{17}$	2.76	$O_4\cdots B_{24}$	3.23
$C_1\cdots C_{22}$	2.83	$C_3\cdots C_{22}$	3.24
$C_3\cdots B_{28}$	2.84	$O_1\cdots B_{17}$	3.29
$C_4\cdots C_{11}$	2.84	$O_3\cdots B_{27}$	3.31
$C_4\cdots C_{12}$	2.87	$O_2\cdots B_{14}$	3.33
$C_2\cdots B_{18}$	2.92	$O_1\cdots B_{18}$	3.37
$C_1\cdots C_{21}$	3.00	$O_4\cdots B_{28}$	3.40
$C_1\cdots B_{18}$	3.02	$C_4\cdots C_{21}$	3.40
$C_4\cdots B_{28}$	3.06		

(b) Intramolecular Contacts Less Than 3.00 Å Involving Hydrogen

Atoms	Dist, Å	Atoms	Dist, Å
$H_{17}\cdots H_{21}$	2.11	$O_6\cdots H_{17}$	2.76
$H_{12}\cdots H_{24}$	2.15	$C_1\cdots H_{17}$	2.50
$H_{12}\cdots H_{21}$	2.39	$C_1\cdots H_{21}$	2.85
$O_1\cdots H_{17}$	2.75	$C_1\cdots H_{22}$	2.52
$O_1\cdots H_{18}$	2.96	$C_2\cdots H_{14}$	2.30
$O_1\cdots H_{22}$	2.38	$C_3\cdots H_{27}$	2.35
$O_2\cdots H_{14}$	2.71	$C_3\cdots H_{28}$	2.89
$O_3\cdots H_{27}$	2.72	$C_4\cdots H_{11}$	2.55
$O_4\cdots H_{11}$	2.36	$C_4\cdots H_{12}$	2.65
$O_4\cdots H_{24}$	2.61	$C_4\cdots H_{24}$	2.46
$O_5\cdots H_{18}$	2.76		

(c) Intermolecular Contacts Less Than 3.60 Å Not Involving Hydrogens[a]

Atoms		Dist, Å	Atoms		Dist, Å
$Cs_1\cdots O_5$	1000	3.12	$O_1\cdots C_6$	2010	3.49
$Cs_1\cdots O_4$	$1\bar{1}00$	3.39	$O_1\cdots O_6$	1000	3.52
$Cs_1\cdots O_6$	1000	3.31	$O_2\cdots O_2$	2011	3.52
$Cs_2\cdots O_6$	1000	3.11	$O_2\cdots C_6$	1000	3.55
$Cs_2\cdots O_5$	1000	3.14	$O_3\cdots O_5$	2010	3.48
$Cs_2\cdots O_1$	1000	3.20	$O_6\cdots B_{17}$	1000	3.44
$Cs_2\cdots O_3$	2010	3.21	$O_6\cdots B_{211}$	1000	3.60
$Cs_2\cdots O_2$	2010	3.58			

(d) Intermolecular Contacts Less Than 3.00 Å Involving Hydrogen

Atoms		Dist, Å	Atoms		Dist, Å
$Cs_1\cdots H_{24}$	1100	2.96	$O_4\cdots H_{211}$	1001	2.67
$Cs_2\cdots H_{151}$	1001	2.99	$O_3\cdots H_{28}$	2110	2.88
$O_6\cdots H_{29}$	1100	2.69	$O_2\cdots H_{14}$	2011	2.91
$H_{21}\cdots H_{26}$	2000	2.44	$H_{12}\cdots H_{16}$	2001	2.23
$H_{16}\cdots H_{26}$	1001	2.21	$H_{19}\cdots H_{212}$	$110\bar{1}$	2.32

[a] Distances are between atom 1 at *x*, *y*, *z* and atom 2 in the symmetry position indicated by the first digit of the four-digit code augmented, in *x*, *y*, and *z*, respectively, by the translations indicated by the next three digits. Symmetry position 1 is *x*, *y*, *z*; position 2 is $\bar{x}$, $\bar{y}$, $\bar{z}$.

are markedly asymmetric with two of the Fe–C bonds being significantly longer than the other two. A similar asymmetry has been inferred[14] in the parent carbonyl $Fe_3(CO)_{12}$ and has been discussed by Dahl in that case and also[15] for the much more asymmetric bridging groups found in the anion $Fe_4(CO)_{13}^{2-}$. In the present case it seems reasonable to suppose that the asymmetry is induced in an inherently labile system so as to reduce intramolecular repulsions between the bridging carbonyl groups and the hydrogen atoms of the icosahedra as may be deduced from Figure 3 and Table V. The distortions are such as to retain an equivalent environment for each iron atom.

Each $Fe_2(CO)$ group in the bridge is planar within the limits of experimental error but the two planes are inclined to one another so as to make an angle of 164° about the Fe–Fe axis. This arrangement is similar to that found in the *cis* isomer of bis(cyclopentadienyldicarbonyliron)[8] where the angle is 164°, in $(C_{10}H_8)_2Fe_4(CO)_{10}$ where an angle of 154° 40′ is noted,[12] and in $[(\pi\text{-}C_5H_5)_2Fe_2(CO)_3]_2P(C_6H_5)_2CCP(C_6H_5)_2$ with an angle of 160°.[16] Again this distortion must serve to relieve stress between the icosahedra and the carbonyl groups. It is absent from the structure of the *trans* isomer of $[\pi\text{-}C_5H_5Fe(CO)_2]_2$ where the crystallographically imposed C_i symmetry requires a planar $Fe_2(CO)_4$ unit.[7,12b]

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[14] C. H. Wei and L. F. Dahl, *J. Amer. Chem. Soc.*, **91**, 1351 (1969).

[15] R. J. Doedens and L. F. Dahl, *ibid.*, **88**, 4847 (1966).

[16] A. J. Carty, T. W. Ng, W. Carter, G. Palenik, and T. Birchall, *Chem. Commun.*, *D*, 1101 (1969).

The terminal Fe–C distances compare reasonably with those found in other complexes involving both bridging and nonbridging carbonyl groups attached to the same iron atom. Thus, an average value of 1.72 Å is given for this bond type[15] in the anion $Fe_4(CO)_{13}^{2-}$. Each Fe–C–O system is linear within the limits of error. There are no significant differences between the four C–O bond distances and the average value of 1.17 Å is normal for this bond.

The five-membered ring of each dicarbollide cage attached to the iron atom is planar. The distances from iron to the center of gravity (cg) of the ring are equivalent and 0.09 Å longer than the corresponding distance in π-$C_5H_5FeB_9C_2H_{11}$[3] and in $Co(B_9C_2H_{11})_2$.[5] This leads to similarly enlarged Fe–C and Fe–B bond distances averaging 2.129 (7) and 2.174 (8) Å, respectively. These distances and the fact that the ring is perpendicular to the axis Fe–cg in each case indicate that the bonding to the rings is symmetrical. The Fe–C distances compare well with the average value of 2.12 Å observed[8] for *cis*-[π-$C_5H_5Fe(CO)_2$]$_2$ and are somewhat shorter than the mean value of 2.15 Å noted[16] in $[(\pi\text{-}C_5H_5)_2Fe_2(CO)_3]_2P(C_6H_5)_2CCP(C_6H_5)_2$. They do not differ significantly from the values observed[7,12b] in *trans*-[π-$C_5H_5Fe(CO)_2$]$_2$. This similarity of bond length is remarkable when compared with the considerable distortion of the whole bonded ring system compared to the latter compound. Thus, the angles Fe–Fe–cg are opened from 120°[17] to 140 and 142°, greater even than the corresponding values of 135° found in the cyclopentadienyl analog.[8] This opening is certainly caused by mutual repulsions between hydrogen atoms on the cages, but it is remarkable that the whole bonded system moves as a rigid body in this distortion maintaining symmetrical bonding to the metal atom.

The exact extent of the repulsions between the hydrogen atoms and other atoms of the molecule is hard to determine. If Figure 3 is taken at face value, then contacts less than the sum of the appropriate van der Waals radii occur between H_{12} and H_{24} and between H_{17} and H_{21} as well as between H_{11} and O_4 and H_{22} and O_1. However, these contacts are based on a model which places the hydrogen atoms on the extensions of the pseudo-fivefold axes of the icosahedra. This assumption is correct for the hydrogen atoms on the side of the polyhedron farthest from the iron atom, but it is probably too radical for the hydrogen atoms attached to the five-membered ring bonded to iron. Here, because of the repulsions with the metal orbitals, the hydrogen atoms are probably displaced toward the plane of the ring. If they are assumed to lie in the ring plane, then *no* intraicosahedral contacts less than, or equal to, the sum of the appropriate van der Waals radii occur. Clearly, the actual structure lies between these two extremes but, unhappily, our experimental data do not allow us to be exact as to where. Most probably the hydrogen atoms are situated so as to give H···H contacts of about 2.4 Å and H···O approaches of about 2.6 Å. The only source of strain would then be in the angle at the iron atom between the orbitals directed at the ring plane and those directed at the carbonyl groups, and if a somewhat "bent" bond is postulated[18] between the halves of the molecule, then even this strain may not be too severe. Figure 3, then, should not be taken too literally; it serves only as a guide to which atoms are in contact in the actual structure.

TABLE VI
RMS AMPLITUDES OF VIBRATION ALONG THE PRINCIPAL AXES OF THE THERMAL ELLIPSOIDS OF THE METAL ATOMS (Å)

Atom	Axis 1	Axis 2	Axis 3
Cs_1	0.238	0.223	0.173
Cs_2	0.237	0.220	0.175
Fe_1	0.169	0.154	0.135
Fe_2	0.175	0.151	0.133

Within the dicarbollyl polyhedra the mean of the 36 independent measurements of the B–B bond distance is 1.787 Å with an rms deviation of 0.027 Å and a standard deviation in the mean of 0.005 Å. This is in good agreement with the mean value of 1.782, rms 0.02 Å, quoted[19] for the anion $[(B_9C_2H_{11})Co]_2(B_8C_2H_{10})^{2-}$. The mean of 12 independent measurements of the B–C bond length is 1.721 (8) Å, rms 0.028 Å, compared to the value of 1.707 Å, rms 0.02 Å, given for the cobalt anion. The mean B–B–B angle based on 60 independent measurements is 60.1 (1)°, rms 1°. The rms deviations from the mean values are somewhat larger than the esd's of the individual values given in Table III. Although it is not to be excluded that there are significant differences in the individual values of the B–B bond distances across the icosahedron, it is more likely that the esd's calculated from the least-squares matrices are underestimated both because of residual systematic errors in the data and because of the use of the block-diagonal approximation.

The cesium cations are loosely and irregularly coordinated by the oxygen atoms of the solvent molecules and approach the oxygen atoms of the carbonyl groups though not sufficiently closely to be thought coordinated to them. The high thermal parameters of the atoms of the acetone and water of solvation indicate that they are not tightly bound in the lattice structure and the unusual occurrence of two different solvent molecules in the crystal is indicative of the difficulty involved in packing together ions of such different sizes.

The thermal behavior of the atoms of the anion is interesting in that the isotropic *B* values of the atoms of the polyhedra are quite small indicating that the cages are firmly bound together and executing a minimum of thermal motion. The rms amplitudes of vibration along the principal axes of the thermal ellipsoids representing the metal atoms are given in Table VI.

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