Crystal and Molecular Structure of Octacarbonyl-μ-[1,2-bis(dimethylarsino)-3,3,4,4,-tetrafluorocyclobutene]-dimanganese (*Mn–Mn*)

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Crystals of the title compound are orthorhombic, space group $Pna2_1$, with $Z = 4$ in a unit cell of dimensions: $a = 17.479(3)$, $b = 10.273(3)$, and $c = 12.713(3)$ Å, with one molecule in the asymmetric unit. The structure was determined from three-dimensional *X*-ray data collected by counter methods and refined by full-matrix least-squares techniques to *R* 3·5% for 1439 observed reflexions. Each manganese atom is bonded to an arsenic atom, four carbonyl groups, and a manganese atom [Mn–Mn 2·971(2), mean Mn–As 2·404(3) Å]. The molecule is twisted about the Mn–Mn bond such that the co-ordinated groups normal to the bond vector are staggered.

THE title compound has been prepared[1] by the reaction of 1,2-bis(dimethylarsino)tetrafluorocyclobutene, $(Me_2As)\overline{C{:}C(AsMe_2){\cdot}CF_2{\cdot}CF_2}$, ($f_4$fars), with decacarbonyldimanganese. From ^{19}F n.m.r. studies of the compound it was predicted to have a Mn–Mn bond and that the $f_4$fars ligand would act as a bridge between the two manganese atoms. Reaction of this compound with iodine at room temperature produced ($f_4$fars)$[Mn(CO)_4I]_2$[2] with rupture of the metal–metal bond. Here we report the result of a detailed structure determination of ($f_4$fars)$[Mn(CO)_4]_2$ in which the effect of displacement of two carbonyl groups by the ligand is examined and the structure is compared with that found for Mn_2CO_{10}. Preliminary results have already been published.[2]

EXPERIMENTAL

A single, orange-coloured crystal of the compound was used in preliminary photographic investigation. Weissenberg (0*kl*, 1*kl* zones) and precession (*h*0*l*, *hk*0 zones) photographs indicated the systematic absences 0*kl* $k + l = 2n + 1$, and *h*0*l* $h = 2n + 1$, which were consistent with the orthorhombic space groups $Pna2_1$ and *Pnam*. A near cube-shaped crystal of edge *ca.* 0·5 mm was very slowly ground to an approximate sphere (diameter 0·36 mm) and then mounted in a general orientation for data collection.

Crystal Data.—$C_{16}H_{12}As_2F_4Mn_2O_8$, $M = 668$, Orthorhombic, $a = 17.479(3)$, $b = 10.273(3)$, $c = 12.713(3)$ Å, $U = 2282.7$ Å^3, $D_m = 1.969$ (Berman density balance, with alcohol as immersion liquid), $Z = 4$, $D_c = 1.945$, $F(000) = 1688$. Mo-K_α radiation, $\lambda = 0.7107$ Å; μ(Mo-K_α) = 23·7 cm^{-1}. Space group $Pna2_1$.

Cell dimensions and intensity data were measured on a computer-controlled Picker four-circle diffractometer by use of the Vanderbilt system. Cell dimensions were determined by a least-squares method using 15 general reflexions whose positions were accurately measured with Mo-$K_{\alpha1}$ radiation (0·70926 Å) with a take-off angle of 0·7°. A unique set of reflexion data was collected by use of niobium-filtered Mo-K_α radiation and a take-off angle of 4·3° with a symmetric θ—2θ scan at 2° min^{-1} of 1·5° width in 2θ (extended to cover the $\alpha_1 - \alpha_1$ splitting). Data for an inner sphere of reflexions ($2\theta < 30°$) were collected with background counts of 10 s at each scan limit; this period was increased to 20 s for the outer ranged data ($30° < 2\theta < 45°$). Three standard reflexions were measured every 4 h (or less) and showed a fluctuation of $\pm 2.3\%$ over the entire data collection. Of the 1580 intensities recorded, 1439 were $> 2.0\sigma$ and were considered observed (σ was taken as $\sqrt{N}$ where *N* is the scan count plus the normalized total of the background counts). Lorentz and polarization factors were applied to give structure-factor moduli.

Structure Determination.—Inspection of the three-dimensional Patterson function yielded two arsenic and two manganese atomic positions in the space group $Pna2_1$. Two cycles of full-matrix least-squares with refinement of scale and atomic parameters gave *R* 0·20. An electron-density synthesis revealed all the remaining non-hydrogen atom positions and *R* was reduced to 0·157. Further least-squares refinement of co-ordinate and isotropic temperature factors for all atoms lowered *R* to 0·065. An electron-density difference map showed anisotropic motion about the two arsenic atoms as the outstanding feature and refinement including these new variables led to *R* 0·055. A subsequent electron-density difference map revealed the positions of all twelve hydrogen atom of the methyl groups and also indicated anisotropic thermal motion about the manganese, fluorine, and oxygen atoms. Inclusion of the hydrogen atoms and refinement of all other co-ordinate and thermal motion parameters reduced *R* to 0·038.

At this stage, the other enantiomorph (with *z* changed to $-z$) was considered. The *R* factor improved to 0·035 with an overall increase in consistency among the As–C bond lengths. The improvement was significant * showing that

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* The *R* factor ratio was 1·086 (1, 1439, 0·01) as compared to the listed value of 1·007 (1, 480, 0·01) according to Hamilton's criterion.[3]

[1] J. P. Crow, W. R. Cullen, and F. L. Hou, personal communication.

[2] J. P. Crow, W. R. Cullen, F. L. Hou, L. Y. Y. Chan, and F. W. B. Einstein, *Chem. Comm.*, 1971, 1229.

[3] W. C. Hamilton, 'Statistics in Physical Science,' Ronald Press, New York, 1964.

this was the correct isomer. The weighting scheme used during the final stages of refinement was $w = 1/\sigma^2$ where $\sigma = \sqrt{1{\cdot}93}$ for $27{\cdot}3 < F_o \leqslant 86{\cdot}3$, $\sigma = (1{\cdot}93)^{\frac{1}{2}}27{\cdot}3/F_o$ for $27{\cdot}3 \geqslant F_0$, and $\sigma = (1{\cdot}93F_0/86{\cdot}3)^{\frac{1}{2}}$ for $86{\cdot}3 < F_0$. A final electron-density difference map showed no variations $> \pm 0{\cdot}39$ eÅ^{-3} (σ 0·20 eÅ^{-3}), the largest peak being 1·38 and 1·56 Å away from O(8) and H(32), and largest trough 0·990 and 0·724 Å from the F(4) and C(16) atoms.

In the calculation of structure factors, atomic scattering factors for hydrogen were taken from ref. 4, and for all other atoms from ref. 5. For As and Mn the Thomas–

TABLE 1

Positional and thermal parameters

Atom	x	y	z	B/Å^2
As(1)	0·3109(1)	0·3287(1)	0·7500	*
As(2)	0·4472(1)	0·1461(1)	0·9574(1)	
Mn(1)	0·2568(1)	0·1160(2)	0·7753(2)	
Mn(2)	0·3994(1)	−0·0182(1)	0·8417(2)	
F(1)	0·3720(5)	0·6069(7)	0·9118(8)	
F(2)	0·4590(5)	0·5767(7)	0·7918(8)	
F(3)	0·5493(5)	0·4584(8)	0·9338(9)	
F(4)	0·4621(6)	0·4838(8)	1·0528(7)	
O(1)	0·1039(5)	0·2143(11)	0·7203(9)	
O(2)	0·2403(6)	0·1783(10)	1·0027(7)	
O(3)	0·1840(6)	−0·1402(10)	0·8086(11)	
O(4)	0·2957(6)	0·0493(11)	0·5544(8)	
O(5)	0·5367(6)	−0·1729(10)	0·8869(9)	
O(6)	0·3121(6)	−0·1333(9)	1·0202(8)	
O(7)	0·3452(6)	−0·2245(8)	0·6995(8)	
O(8)	0·4672(5)	0·1188(8)	0·6592(8)	
C(1)	0·1649(7)	0·1792(13)	0·7401(12)	4·4 †
C(2)	0·2498(7)	0·1521(11)	0·9153(9)	3·3
C(3)	0·2140(7)	−0·0405(13)	0·7977(11)	4·8
C(4)	0·2825(7)	0·0728(12)	0·6404(11)	4·0
C(5)	0·4838(7)	−0·1093(12)	0·8691(10)	4·2
C(6)	0·3433(7)	−0·0851(11)	0·9507(11)	3·9
C(7)	0·3657(6)	−0·1424(11)	0·7555(10)	3·9
C(8)	0·4379(6)	0·0691(11)	0·7311(9)	3·3
C(9)	0·2376(7)	0·4736(12)	0·7704(9)	5·0
C(10)	0·3600(8)	0·3812(14)	0·6200(11)	4·9
C(11)	0·5577(7)	0·1461(12)	0·9710(12)	4·6
C(12)	0·4151(8)	0·1570(13)	1·1053(11)	5·0
C(13)	0·3881(6)	0·3859(10)	0·8477(10)	3·2
C(14)	0·4334(6)	0·3249(12)	0·9169(9)	3·7
C(15)	0·4216(7)	0·5180(14)	0·8693(11)	4·8
C(16)	0·4736(8)	0·4501(14)	0·9500(13)	5·5
H(11)	0·275	0·515	0·750	‡
H(12)	0·221	0·436	0·706	
H(13)	0·225	0·450	0·830	
H(21)	0·404	0·342	0·600	
H(22)	0·370	0·485	0·630	
H(23)	0·330	0·345	0·570	
H(31)	0·565	0·200	1·019	
H(32)	0·565	0·047	0·988	
H(33)	0·571	0·145	0·570	
H(41)	0·361	0·189	1·084	
H(42)	0·422	0·076	1·113	
H(43)	0·448	0·211	1·138	

Anisotropic thermal parameters ($U \times 10^4$ Å^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
As(1)	386(6)	342(5)	349(7)	23(5)	−40(6)	68(6)
As(2)	378(6)	347(5)	310(6)	26(5)	−50(6)	21(6)
Mn(1)	374(8)	429(9)	407(10)	−4(7)	−21(8)	−15(8)
Mn(2)	483(9)	325(8)	389(9)	34(8)	10(8)	8(9)
	U $\times 10^3$ (A^2)					
F(1)	116(7)	40(4)	137(9)	17(5)	−28(6)	−28(5)
F(2)	117(7)	55(5)	118(8)	−30(5)	−13(6)	23(5)
F(3)	67(5)	70(5)	152(9)	−9(5)	−31(6)	−9(5)
F(4)	142(9)	69(6)	81(6)	−2(6)	−43(6)	−30(5)
O(1)	52(6)	117(9)	101(9)	21(6)	−15(6)	−7(7)
O(2)	87(7)	102(8)	41(5)	15(6)	13(5)	−4(5)
O(3)	94(8)	71(7)	144(12)	−36(6)	20(8)	−3(7)
O(4)	95(7)	117(8)	45(5)	28(7)	00(5)	−30(6)
O(5)	75(7)	84(7)	96(8)	48(6)	−28(6)	−10(6)
O(6)	91(7)	71(6)	71(6)	4(6)	29(6)	14(6)
O(7)	113(8)	47(5)	63(6)	−7(5)	−16(6)	−8(5)
O(8)	80(6)	62(6)	59(5)	−12(5)	17(5)	3(5)

* Anisotropic temperature parameters. † Standard errors for the isotropic thermal parameters of the C atoms are 0·3 Å^2. ‡ Temperature factors for the hydrogen are 7·25 Å^2.

TABLE 2

Interatomic distances and angles

(*a*) Bonded distances (Å)

Mn(1)–Mn(2)	2·971	C(13)–C(14)	1·34
Mn(1)–As(1)	2·405 *	C(13)–C(15)	1·50
Mn(2)–As(2)	2·392 *	C(14)–C(6)	1·53
Mn(1)–C(1)	1·79	C(15)–C(16)	1·54
Mn(1)–C(2)	1·79	C(15)–F(1)	1·37
Mn(1)–C(3)	1·83	C(15)–F(2)	1·33
Mn(1)–C(4)	1·80	C(16)–F(3)	1·34
Mn(2)–C(5)	1·79	C(16)–F(4)	1·37
Mn(2)–C(6)	1·78	C(1)–O(1)	1·15
Mn(2)–C(7)	1·83	C(2)–O(2)	1·15
Mn(2)–C(8)	1·80	C(3)–O(3)	1·16
As(1)–C(9)	1·98	C(4)–O(4)	1·14
As(1)–C(10)	1·94	C(5)–O(5)	1·16
As(1)–C(13)	1·93	C(6)–O(6)	1·15
As(2)–C(11)	1·94	C(7)–O(7)	1·16
As(2)–C(12)	1·96	C(8)–O(8)	1·16
As(2)–C(14)	1·93	$0{\cdot}82 \leqslant$ C–H $\leqslant 1{\cdot}09$	

Standard errors in bond lengths are: 0·002 Mn–Mn, Mn–As; 0·02 Å Mn–C, As–C, C–C, C–F, and C–O.

* Corrected for thermal riding motion of the As on the Mn atoms. The uncorrected values are 2·403 and 2·389 Å.

(*b*) Bond angles (°)

As(1)–Mn(1)–Mn(2)	97·44	As(2)–Mn(2)–Mn(1)	98·05
As(1)–Mn(1)–C(1)	89·4	As(2)–Mn(2)–C(5)	87·8
As(1)–Mn(1)–C(2)	88·4	As(2)–Mn(2)–C(6)	89·2
As(1)–Mn(1)–C(3)	177·9	As(2)–Mn(2)–C(7)	178·9
As(1)–Mn(1)–C(4)	90·0	As(2)–Mn(2)–C(8)	89·9
Mn(2)–Mn(1)–C(1)	171·6	Mn(1)–Mn(2)–C(5)	173·8
Mn(2)–Mn(1)–C(2)	84·5	Mn(1)–Mn(2)–C(6)	86·5
Mn(2)–Mn(1)–C(3)	84·7	Mn(1)–Mn(2)–C(7)	83·1
Mn(2)–Mn(1)–C(4)	88·3	Mn(1)–Mn(2)–C(8)	81·9
C(1)–Mn(1)–C(2)	96·3	C(5)–Mn(2)–C(6)	95·6
C(1)–Mn(1)–C(3)	89·5	C(5)–Mn(2)–C(7)	91·0
C(1)–Mn(1)–C(4)	94·2	C(5)–Mn(2)–C(8)	96·1
C(2)–Mn(1)–C(3)	90·0	C(6)–Mn(2)–C(7)	91·1
C(2)–Mn(1)–C(4)	169·3	C(6)–Mn(2)–C(8)	168·2
C(3)–Mn(1)–C(4)	91·9	C(7)–Mn(2)–C(8)	90·0
Mn(1)–As(1)–C(9)	114·3	Mn(2)–As(2)–C(11)	113·7
Mn(1)–As(1)–C(10)	122·8	Mn(2)–As(2)–C(12)	101·5
Mn(1)–As(1)–C(13)	117·8	Mn(2)–As(2)–C(14)	117·8
C(9)–As(1)–C(10)	100·8	C(11)–As(2)–C(12)	101·5
C(9)–As(1)–C(13)	98·0	C(11)–As(2)–C(14)	98·6
C(10)–As(1)–C(13)	98·9	C(12)–As(2)–C(14)	99·6
C(13)–C(15)–C(16)	86·1	C(14)–C(16)–C(16)	85·8
F(1)–C(15)–F(2)	107·6	F(3)–C(16)–F(4)	105·9
F(1)–C(15)–C(13)	115·3	F(3)–C(16)–C(14)	117·8
F(1)–C(15)–C(16)	114·4	F(3)–C(16)–C(15)	116·9
F(2)–C(15)–C(13)	117·8	F(4)–C(16)–C(14)	114·2
F(2)–C(15)–C(16)	114·2	F(4)–C(16)–C(15)	115·9

Standard errors in angles are:

As–Mn–Mn 0·06; As–Mn–C, Mn–As–C, and Mn–Mn–C 0·4; C–As–C 0·6; C–C–C 1·0; F–C–C $\leqslant 1{\cdot}3$; F–C–F $\leqslant 1{\cdot}2$; Mn–C–O $\leqslant 1{\cdot}4$.

Mn(1)–C(1)–O(1)	176·2	Mn(2)–C(6)–O(6)	175·2
Mn(1)–C(2)–O(2)	175·3	Mn(2)–C(7)–O(7)	178·6
Mn(1)–C(3)–O(3)	176·9	Mn(2)–C(8)–O(8)	174·8
Mn(1)–C(4)–O(4)	176·8	C(13)–C(14)–C(16)	93·3
Mn(2)–C(5)–O(5)	177·2	C(14)–C(13)–C(15)	94·2

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[4] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 1965, **42**, 3175.

[5] 'International Tables for *X*-Ray Crystallography,' vol. 3, Kynoch Press, Birmingham, 1965, 3.3.

TABLE 2 (*Continued*)

(*c*) Selected intramolecular non-bond contacts (Å)

As(1) · · · As(2)	4·018	C(1) · · · C(2)	2·69
As(1) · · · Mn(2)	4·057	C(1) · · · C(3)	2·52
As(1) · · · C(1)	2·98	C(1) · · · C(4)	2·65
As(1) · · · C(2)	2·98	C(5) · · · C(6)	2·54
As(1) · · · C(4)	3·02	C(5) · · · C(7)	2·68
		C(5) · · · C(8)	2·66
As(2) · · · Mn(1)	4·065		
As(2) · · · C(5)	2·93		
As(2) · · · C(6)	2·99	C(2) · · · C(6)	2·97
As(2) · · · C(8)	3·00	C(3) · · · C(6)	3·02
		C(3) · · · C(7)	2·90
F(1) · · · F(2)	2·18	C(4) · · · C(7)	3·02
F(1) · · · F(3)	2·70	C(4) · · · C(8)	2·95
F(1) · · · F(4)	3·18		
F(2) · · · F(3)	2·69		
F(2) · · · F(4)	3·39		
F(3) · · · F(4)	2·16		

(*d*) Intermolecular non-hydrogen contacts ($<$3·3 Å)

F(3) · · · C(10^{I})	3·29	O(2) · · · O(7^{III})	3·08
O(1) · · · O(8^{II})	3·04	O(6) · · · C(10^{III})	3·27

Roman numerals as superscripts refer to the following equivalent positions relative to the reference molecule at x, y, z:

I $1 - x, 1 - y, \frac{1}{2} + z$
II $x - \frac{1}{2}, \frac{1}{2} - y, z$
III $\frac{1}{2} - x, \frac{1}{2} + y, z - \frac{1}{2}$

Fermi–Dirac model with full allowance for anomalous scattering was used. The programs used are listed in ref. 6.

Table 1 gives the final atomic parameters. Table 2 lists interatomic distances and angles. Errors were estimated by the least-squares procedures, and are given in parentheses and include both correlation effects and cell-dimension errors, where appropriate. Table 3 summarizes the equations for relevant mean planes. Figure 1 shows a diagram of the molecular structure with the atom numbering system used, and Figure 2 shows the crystal packing. Final observed and calculated structure factors are listed in Supplementary Publication No. SUP 20537 (4 pp., 1 microfiche).*

TABLE 3

Mean planes. Equations of planes are in the form $lx + my + nz + p = 0$ and co-ordinates are referred to axes of the unit cell in Å

	l	m	n	p	χ^2
Plane (1):					
C(13)—(16)	0·6849	−0·1465	−0·7137	−3·6240	0·27
Plane (2):					
As(1), As(2), C(1), C(3)	0·1840	−0·2326	−0·9550	−8·8911	0·66
Plane (3):					
As(1), As(2), C(13), C(14)	0·6988	−0·1074	−0·7072	−3·3079	0·02
Plane (4):					
As(1), As(2), C(13)—(16)	0·6923	−0·1215	−0·7113	−3·4301	11·04

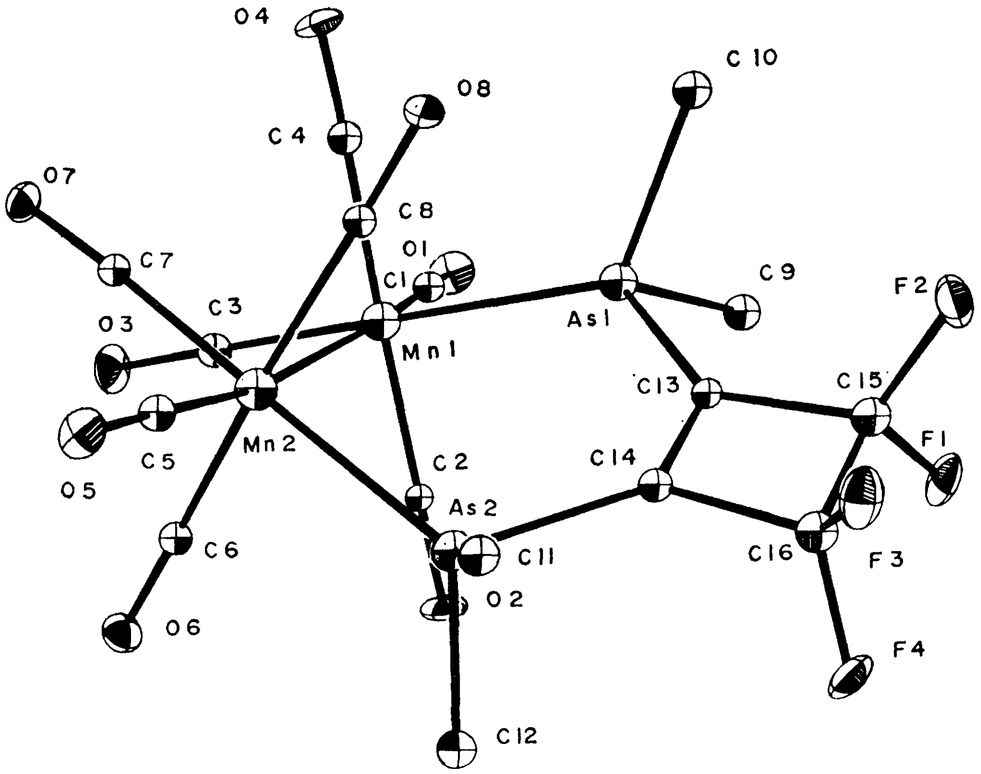

FIGURE 1 Molecular structure; the thermal ellipsoids (except those for the arsenic and manganese atoms which were given isotropic values) are drawn to scale and contain 8% of the electron density

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* For details see Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), 1970, Issue No. 20 (items less than 10 pp. are sent as full size copies).

[6] L. Y. Y. Chan and F. W. B. Einstein, *Canad. J. Chem.*, 1971, **46**, 487.

RESULTS AND DISCUSSION

The $f_4farsMn_2(CO)_8$ molecule consists of two manganese atoms each in a distorted octahedral environment comprised of four carbonyl groups, an arsenic atom, and a Mn–Mn bond. The molecule has an approximate noncrystallographic two-fold axis of symmetry, which passes through the mid-points of the Mn–Mn and As $\cdots$ As vectors. The structure is therefore similar to that found[7] for $Mn_2(CO)_{10}$ with an arsenic atom replacing a carbonyl group on each manganese atom. The octahedra are almost perfectly staggered even though the ligand bridges the Mn–Mn bond. The Mn–Mn bond in this case, however, is substantially longer [2·971(2) compared to 2·923(3) Å in $Mn_2(CO)_{10}$], although in both cases the Mn–Mn bonds are longer than twice the covalent radius for Mn (1·39—1·43 Å).[8] The long Mn–Mn bond in $Mn_2(CO)_{10}$ had been attributed to the negative charge localized on the metal atoms through co-ordination with the CO ligands[7] and to an increase in the p and d character in the orbital directed along the metal–metal σ bond.[9] The situation in the $f_4$fars derivative is similar but, in addition, the arsenic atom is probably a better σ donor and a less efficient π acceptor to the Mn atom compared with a carbonyl group. Consequently, the increased repulsion between the Mn atoms owing to this increased effective negative charge may lead to the longer Mn–Mn bond.

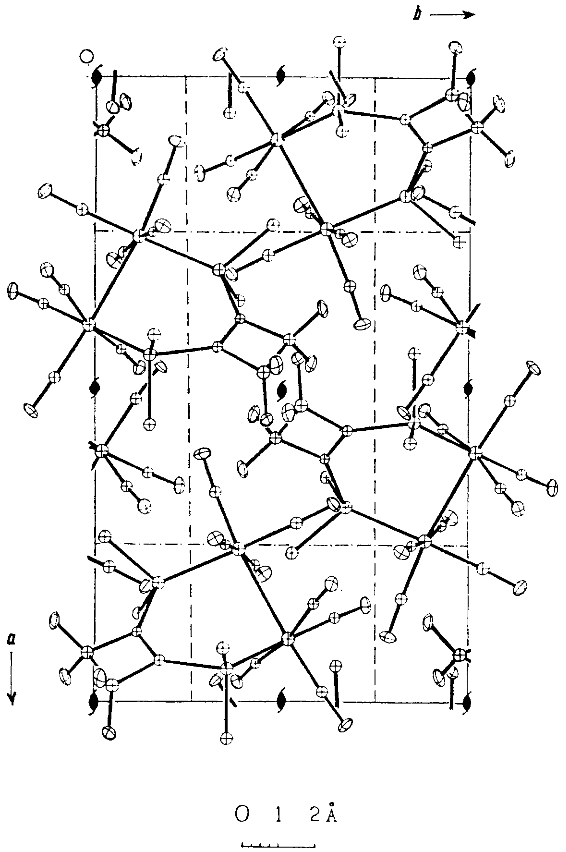

FIGURE 2 Crystal structure viewed down the c axis

The two sets of carbon atoms, C(2)—(4) and C(6)—(8), are bent towards each other as seen from the angles (all are less than 90°) they make with the Mn–Mn bond vector. As in $Mn_2(CO)_{10}$, the geometry results from the repulsive forces between these carbon atoms and the terminal carbon atoms C(1) and C(5) respectively, as suggested by their non-bonded contacts. The arsenic atoms, however, are bent outwards from the Mn–Mn bond; the mean Mn–Mn–As angle being 97·7° and with a mean Mn–As bond length of 2·404 Å, a bite of 4·017(3) Å across the arsenic–arsenic atoms is maintained. This bite of the $f_4$fars ligand has been found to depend largely on the mode of ligation, for instance, it is 3·233 Å in $(f_4fars)Fe_2(CO)_6$[10] where the $f_4$fars is a chelate, 4·108 Å in $(f_4fars)_2Ru_3(CO)_8$[11] where each $f_4$fars ligand bridges two Ru atoms which are also linked by a metal–metal bond as in the present compound, and 4·31 Å in $(f_4fars)Mn_2(CO)_8I_2$[2] where a metal–metal bond is not present and the $f_4$fars ligand provides the only linkage between the two $Mn(CO)_4I$ units.

The arsenic atoms and the cyclobutene ring are planar. All As–C bonds are essentially equivalent (within the limits of our errors). For the cyclobutene ring, the C(13)–C(14) bond is 1·34(2) Å, close to the expected value.[12] The remaining C–C bonds are significantly longer [1·51—1·55(2) Å] and correspond to C–C single-bond values. The C–C–C angles in the ring differ from 90° in the direction imposed by the double bond. The C–F bonds (mean 1·35 Å) compare well with those found in other compounds containing the $f_4$fars ligand.

The Mn–C and C–O bonds range from 1·77—1·86 and 1·14—1·17 Å respectively. Variations in these distances are not significant. All the Mn–C–O angles are linear.

The thermal motion of each of the oxygen atoms is mainly perpendicular to the appropriate corresponding bond vectors. The major thermal motion of the fluorine atoms is oblique to the C–F bond vectors. While the major direction of motion of the arsenic atoms is approximately perpendicular to the As–Mn bonds, that of the Mn atoms almost bisects the As–Mn–Mn angles. No correction for anisotropic motion was made to any bonds involving light atoms.

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