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The Crystal Structure of Dimanganese Decacarbonyl, $Mn_2(CO)_{10}$

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$Mn_2(CO)_{10}$ crystallizes with four molecules per unit cell in space group $I2/a$ with

$$a = 14\cdot16 \pm 0\cdot02,\ b = 7\cdot11 \pm 0\cdot02,\ c = 14\cdot67 \pm 0\cdot02\ \text{Å};\ \beta = 105 \pm 0\cdot5° .$$

The approximate structure was determined from two-dimensional data by a combination of the heavy atom and isomorphous-replacement techniques (Dahl *et al.*, 1957). The structure has been refined to an R_1 value of 7·0% by the application of an anisotropic least-squares method to the three-dimensional data.

$Mn_2(CO)_{10}$ consists of discrete molecules of approximately D_{4d} symmetry. Each manganese atom is octahedrally coordinated to five carbonyl groups and the other manganese atom in such a way that the equatorial carbonyl groups are arranged in a staggered configuration. The refined distance for the direct Mn-Mn bond is 2·923 Å.

Introduction

The crystallographically isomorphous polynuclear metal carbonyls, $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$, were found from a two-dimensional X-ray study to have approximately D_{4d} molecular symmetry with direct metal–metal bonds and no bridging carbonyl groups (Dahl *et al.*, 1957). The present paper presents the results of a three-dimensional X-ray investigation of $Mn_2(CO)_{10}$.

Experimental procedure

Preparation and properties of $Mn_2(CO)_{10}$

$Mn_2(CO)_{10}$ was prepared by Brimm, Lynch & Sesny (1954) and made available through the generosity of Prof. G. Wilkinson. The preparation consists in reducing manganese(II) iodide with magnesium in diethyl ether at room temperature under a carbon monoxide pressure of 68–200 atmospheres. The pure compound forms golden-yellow, transparent crystals which melt in a sealed tube at 154–155 °C. In the absence of carbon monoxide the crystals begin to decompose at approximately 110 °C. Since the crystals are reactive with air and water, samples were transferred by vacuum sublimation into thin-walled glass capillaries which were then hermetically sealed. Single crystals were formed by resublimation within the sealed capillaries.

Most crystals were unstable in the X-ray beam, presumably due to small amounts of occluded water, and either decomposed after a few days or disintegrated by cleavage along planes perpendicular to the b axis. A crystal was finally isolated which was sufficiently stable to provide the three-dimensional intensity data.

X-ray data

Multiple-film equi-inclination Weissenberg photographs about the b_0 axis involving eight reciprocal layers, $h0l$ through $h7l$, were taken with Zr-filtered Mo $K\alpha$ radiation. Timed-exposure precession photographs of $0kl$ and $hk0$ reciprocal levels were obtained with the same radiation.

The intensities were estimated visually by comparison with a calibrated standard set of intensities prepared from the same crystal. Lorentz-polarization corrections for the precession photographs were made with a template (Waser, 1951). The Weissenberg photographs were corrected for both Lorentz-polarization effects (Zalkin & Jones, 1956) and extension of spots (Phillips, 1954). Since the crystal utilized was small, no absorption correction was applied. Extinction corrections were not made. The combined three-dimensional intensity data consist of 614 independent, observed reflections.

Unit cell and space group

The unit cell is monoclinic with lattice constants

$$a = 14\cdot16 \pm 0\cdot02,\ b = 7\cdot11 \pm 0\cdot02,$$
$$c = 14\cdot67 \pm 0\cdot02\ \text{Å};\ \beta = 105° \pm 0\cdot5°.$$

Four dimeric molecules per unit cell give a calculated density 1·82 g.cm.$^{-3}$ compared with an observed value (Brimm *et al.*, 1954) of 1·75 g.cm.$^{-3}$. The lattice parameters are in reasonable agreement with the values

$$a = 14\cdot16,\ b = 7\cdot16,\ c = 14\cdot68\ \text{Å};\ \beta = 105°,$$

reported by Brimm *et al.* (1954) and with those found by Trueblood & Wallach (1961):

$$a=14{\cdot}18,\ b=7{\cdot}14,\ c=14{\cdot}66\ \text{Å};\ \beta=105°.$$

Systematic absences of hkl reflections for $h+k+l=2n+1$ and $h0l$ reflections for $h=2n+1$ indicate the space groups $I2/a$ (C_{2h}^6) or Ia (C_s^4). The more common C-centered cell, defined by the choice of a diagonal axis as the new a lattice constant, is less convenient because its monoclinic angle is greater. An intensity distribution study (Howells *et al.*, 1950) indicates $I2/a$ as the more probable space group, and the structure found is based on it.

Two-dimensional determination of atomic positions

For the centrosymmetric space group $I2/a$, the diffraction data indicate that the metal, carbon, and oxygen atoms are in the general 8-fold set of positions: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \pm x, y, z; \frac{1}{2}+x, \bar{y}, z$ (*International Tables for X-ray Crystallography*, 1952). This gives 33 positional parameters to be determined corresponding to one manganese, five carbon, and five oxygen atoms in the asymmetric unit. The manganese positional parameters were determined from conventional two-dimensional Patterson projections. Initially, the two-dimensional data were placed on an absolute scale by the application of Wilson's (1942) method. The presence of a heavy atom and the isomorphism of the manganese and rhenium compounds greatly simplified the phase determination for each reflection.

A molecular configuration was obtained from consideration of Fourier projections and difference syntheses. Temperature corrected structure factor calculations for the three principal zones gave a final two-dimensional discrepancy factor,

$$R_1=(\Sigma||F_o|-|F_c||/\Sigma|F_o|)\times 100,$$

of 20·5% for the ($h0l$) zone, 20·0% for the ($hk0$) zone, and 22·2% for the ($0kl$) zone. At this point the gross features of the molecular structure were clear but intimate details were lacking (Dahl *et al.*, 1957).

Three-dimensional least-squares refinement

The first three-dimensional refinement cycles were carried out on an IBM 650 computer (Senko & Templeton, 1956) with individual isotropic temperature parameters and constant weighting factors. The atomic form factors used were those of Berghuis *et al.* (1955) for carbon and oxygen and those of Thomas & Umeda (1957) for manganese. After thirteen cycles of this essentially diagonal least-squares refinement the reliability index had maintained the value of 11·5% for several cycles. However, an examination of the parameter shifts and standard deviations obtained from the thirteenth cycle indicated that many shifts were still significant, particularly that for the y coordinate of the apical oxygen atom O_1. The temperature factor for O_1 was unusually high and still increasing. These facts indicated that the use of a full-matrix least-squares program would be needed for further refinement.

At this time an IBM 704 was made available to us, and the full-matrix least-squares program of Busing & Levy (1959) was employed. After several cycles of isotropic refinement with variable weighting factors (Hughes, 1941; Lavine & Lipscomb, 1954) the reliability index dropped to 10·5%. The final parameters from this isotropic refinement are given in Table 1.

Table 1. *Final parameters with standard deviations from isotropic least-squares refinement on IBM* 704

Atom	x	$10^3\sigma(x)$	y	$10^3\sigma(y)$	z	$10^3\sigma(z)$	B (Å^2)	$\sigma(B)$
Mn	0·1542	0·2	0·2302	0·3	0·9318	0·2	3·0	0·1
C_1	0·0401	1·6	0·2334	3·5	0·8465	1·5	6·0	0·5
O_1	0·9687	1·5	0·2530	3·6	0·7833	1·6	9·7	0·5
C_2	0·1100	1·3	0·3337	2·7	0·0255	1·3	4·1	0·4
O_2	0·0787	1·0	0·3934	2·1	0·0883	1·0	5·6	0·3
C_3	0·2205	1·4	0·1267	2·9	0·8528	1·4	4·6	0·4
O_3	0·2576	1·1	0·0509	2·1	0·8018	1·1	5·8	0·3
C_4	0·1317	1·4	−0·0025	3·0	0·9726	1·4	4·4	0·4
O_4	0·1126	1·1	0·8565	2·4	0·0015	1·2	6·5	0·4
C_5	0·1850	1·3	0·4683	2·6	0·9004	1·3	3·7	0·4
O_5	0·2089	1·0	0·6157	2·2	0·8786	1·0	5·5	0·3

Table 2. *Final positional parameters with standard deviations from anisotropic least-squares refinement on IBM* 704

Atom	x	$10^3\sigma(x)$	y	$10^3\sigma(y)$	z	$10^3\sigma(z)$
Mn	0·1542	0·1	0·2308	0·2	0·9319	0·1
C_1	0·0393	1·0	0·2364	2·5	0·8446	1·0
O_1	0·9675	0·9	0·2438	3·0	0·7859	1·1
C_2	0·1088	0·8	0·3352	2·0	0·0284	1·0
O_2	0·0788	0·7	0·3963	1·6	0·0877	0·7
C_3	0·2190	1·0	0·1226	2·2	0·8523	1·0
O_3	0·2579	0·9	0·0496	1·6	0·8013	0·7
C_4	0·1314	0·9	−0·0005	2·2	0·9732	1·0
O_4	0·1116	0·8	−0·1431	1·6	0·0013	0·8
C_5	0·1862	1·0	0·4667	1·8	0·9007	0·8
O_5	0·2097	0·8	0·6147	1·6	0·8793	0·7

The full-matrix program gave negligible parameter shifts; however, an analysis of the bond lengths and angles together with strong evidence on the (010) difference syntheses of anisotropic thermal motion of the apical carbonyl indicated that an anisotropic refinement was desirable.

Table 3. *Final anisotropic temperature coefficients*

($\text{Å}^2 \times 10^3$)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Mn	38 ± 1	158 ± 4	40 ± 1	−4 ± 2	5 ± 1	28 ± 2
C_1	60 ± 8	334 ± 44	77 ± 9	−18 ± 18	−9 ± 7	25 ± 19
O_1	96 ± 9	694 ± 58	124 ± 11	−21 ± 22	−40 ± 9	53 ± 24
C_2	40 ± 6	280 ± 36	52 ± 8	22 ± 13	−2 ± 6	25 ± 14
O_2	71 ± 6	390 ± 32	63 ± 7	−30 ± 12	32 ± 6	59 ± 12
C_3	70 ± 8	273 ± 38	37 ± 8	−6 ± 15	−2 ± 6	−20 ± 14
O_3	125 ± 9	320 ± 31	63 ± 7	−58 ± 14	52 ± 7	9 ± 11
C_4	41 ± 7	257 ± 36	70 ± 9	12 ± 12	21 ± 7	22 ± 15
O_4	102 ± 8	243 ± 27	91 ± 9	56 ± 13	48 ± 7	16 ± 13
C_5	68 ± 9	164 ± 35	32 ± 6	−14 ± 13	−1 ± 6	2 ± 11
O_5	106 ± 8	239 ± 28	56 ± 6	−11 ± 12	−4 ± 6	10 ± 11

Table 4. *Observed and calculated structure factors*

h	k	l	F_o	F_c
0	0	2	208.8	178.9
		4	45.5	-41.4
		6	77.1	-70.6
		8	79.5	-66.8
		12	18.2	20.6
		14	39.5	40.5
		16	14.6	14.1
2	0	0	124.2	-105.6
		2	138.4	118.5
		4	222.1	194.2
		6	45.9	42.3
		10	53.6	-50.6
		12	43.7	-42.4
		14	20.2	-22.8
		18	12.9	15.1
-2	0	2	209.6	-184.3
		4	55.8	-51.4
		6	15.7	8.0
		8	28.3	29.8
		10	54.7	53.4
		12	61.3	63.1
		16	22.0	-23.9
		18	16.2	-17.7
		20	9.6	-13.3
4	0	0	116.2	-106.3
		2	461.0	-404.7
		4	181.5	-171.8
		6	33.8	37.1
		8	95.3	94.4
		10	32.0	38.7
		16	17.7	-21.8
-4	0	2	67.2	-63.6
		4	82.3	76.9
		6	88.9	82.4
		8	17.1	-17.4
		12	60.7	-60.5
		14	23.2	-22.2
		20	11.8	17.3
6	0	0	61.5	52.0
		2	67.2	64.6
		4	57.5	-53.4
		6	150.5	-144.5
		8	24.3	-24.4
		12	30.9	30.9
		14	26.8	29.7
-6	0	2	47.8	44.0
		4	20.4	22.6
		8	93.1	-91.3
		10	83.3	-85.1
		14	17.7	17.7
		16	27.4	30.9
		18	18.8	22.0
8	0	0	19.3	21.4
		2	87.2	90.9
		4	167.0	148.6
		6	61.9	65.0
		10	52.2	-54.7
		12	28.1	-26.5
		16	9.1	11.1
-8	0	2	56.0	-54.5
		4	58.0	-51.7
		6	26.5	-25.0
		10	63.7	67.1
		12	24.3	19.9
		18	17.3	-21.2
		20	7.4	-9.7
10	0	0	59.6	-61.2
		2	23.2	-21.0
		6	16.2	17.7
		8	61.3	66.5
		10	20.2	22.8
		14	14.0	-20.4
-10	0	2	22.8	-25.2
		4	17.1	12.9
		6	79.5	76.6
		8	66.5	65.5
		10	14.0	14.3
		12	14.6	-12.9
		14	37.8	-41.7
		16	19.8	-21.2
12	0	0	15.6	13.7
		4	40.2	-42.8
		6	54.9	-60.6
		8	21.3	-27.1
		12	19.5	24.4
-12	0	2	55.4	51.9
		4	35.3	36.4
		6	15.6	-16.7
-12	0	8	34.2	-35.2
		10	19.9	-17.9
		12	15.1	-15.6
		14	11.3	12.4
		16	19.0	19.3
		18	11.8	11.9
14	0	0	15.1	16.2
		2	31.4	32.5
		4	20.4	17.6
		10	19.9	-22.3
-14	0	4	41.9	-43.3
		6	41.1	-41.8
		8	13.5	-14.4
		10	11.6	13.7
		12	33.4	34.3
		14	16.0	18.1
16	0	0	28.3	-30.1
		6	18.4	22.2
-16	0	2	16.7	-18.5
		8	16.7	19.0
		14	12.9	-14.3
		16	18.2	-12.9
18	0	2	9.1	-12.1
-18	0	2	19.3	20.9
		4	18.4	19.9
		10	19.5	-22.4
		12	11.3	-14.9
0	1	1	14.6	11.1
-4			73.7	-72.6
-6			38.9	36.8
8			45.9	44.6
-8			48.0	45.6
10			20.8	-23.3
-10			20.1	-24.0
0	1	3	22.3	22.7
2			59.2	58.1
-4			129.4	-140.4
-6			71.7	68.5
0	1	5	137.8	139.5
-2			112.1	-110.4
6			36.8	-33.4
-6			22.9	-15.7
0	1	7	19.5	10.7
2			60.5	57.2
4			49.3	-45.7
0	1	9	30.6	-28.4
2			29.2	30.0
-10			25.7	-18.9
0	1	11	8.3	-13.3
0	1	13	8.3	6.5
0	1	15	11.8	15.9
1	1	0	187.2	-176.6
3			46.6	-44.9
5			112.1	110.6
7			35.5	-36.6
9			42.4	-45.1
11			66.8	68.3
15			27.1	-30.6
3	1	2	123.9	-126.4
5			100.9	104.5
-5			32.0	-28.8
7			34.8	33.1
-7			146.8	144.5
9			87.7	-90.5
-9			31.3	-25.9
-11			68.2	-68.4
-13			32.7	36.3
15			27.1	-31.8
1	1	4	41.0	37.9
-1			34.1	-31.5
3			107.2	-99.4
-3			220.0	-230.8
5			27.8	25.3
7			108.6	109.8
-7			86.2	90.4
9			34.8	-35.9
-9			83.5	-77.8
13			41.7	45.8
-13			53.6	52.5
1	1	6	126.6	128.0
-1			36.8	-38.2
-3			103.0	-107.2
5	1	6	70.2	-68.4
-5			144.7	134.6
7			54.9	52.8
-7			29.2	25.2
-9			73.0	-67.2
11			53.6	-54.0
-11			44.5	44.3
-13			27.8	24.4
-15			26.4	-30.9
1	1	8	84.9	82.2
-1			112.7	-114.5
3			38.9	38.8
5			76.5	-67.3
-5			91.8	88.5
-7			69.6	-62.9
9			35.5	34.3
-9			29.9	-29.6
11			30.6	-35.3
-11			43.8	43.2
-1	1	10	78.6	-76.4
3			79.3	80.6
-3			68.2	64.4
-7			66.8	-63.9
9			32.6	37.2
1	1	12	60.5	-62.3
3			38.9	41.0
-3			57.0	57.5
7			43.8	-40.5
-9			27.8	29.3
-13			30.6	-29.4
1	1	14	36.8	-39.4
5			27.1	33.8
-9			29.9	30.8
-11			26.4	-31.4
0	2	0	139.5	-131.3
2			70.1	-65.0
4			83.2	81.3
6			105.4	-107.5
10			68.7	69.7
12			20.9	-21.6
16			32.7	33.6
0	2	2	64.1	-60.3
4			85.1	83.5
-4			27.5	24.9
-6			59.6	-66.9
8			76.0	-76.7
-8			50.4	48.1
10			51.7	44.4
-10			26.8	26.0
-12			66.1	-65.9
14			44.5	-36.8
2	2	4	93.0	-92.8
-2			82.5	89.3
4			39.9	39.2
-4			65.5	-65.6
6			36.6	35.7
-6			32.1	-32.5
8			62.2	-62.0
-8			94.9	95.3
-10			51.7	-53.2
12			35.4	36.2
-12			43.8	-40.5
-14			47.8	46.1
0	2	6	70.1	68.9
2			76.0	-71.4
-4			110.7	-118.1
6			68.1	67.2
-6			58.9	59.1
-8			50.4	51.0
-10			77.2	-82.2
12			40.6	36.6
-14			42.6	43.2
0	2	8	79.2	73.0
-2			51.0	-51.6
4			66.8	-71.0
-4			56.3	-53.4
6			23.5	22.9
-6			121.2	128.1
10			38.0	-35.8
-10			50.4	-49.5
-12			37.3	35.5
0	2	10	51.7	48.3
2			51.7	51.1
-2			95.6	-105.2
4			43.1	-39.5
-4			30.7	29.4
-6			46.4	47.8
8			37.3	34.7
-8			47.8	-47.1
-12			38.0	41.6
0	2	12	21.6	-23.8
2			64.8	63.7
-2			43.8	-45.2
-4			45.2	45.1
6			30.1	-27.7
-8			52.4	-53.0
-10			34.0	31.9
0	2	14	41.9	-42.9
2			28.1	26.2
-4			43.8	42.5
6			30.7	-33.0
-6			35.4	-33.3
-10			24.9	25.5
0	2	16	20.9	-24.2
-2			20.9	29.3
-6			20.9	-27.9
3	2	1	77.9	82.2
-3			120.5	-143.6
5			24.9	16.6
-5			11.1	1.2
7			60.2	-56.3
-7			26.1	23.6
9			24.2	-17.2
-9			28.8	26.9
-11			17.0	-19.0
1	2	3	136.9	153.4
-1			26.8	-23.5
3			54.3	-54.3
-3			37.3	-38.1
5			18.3	18.7
-5			32.1	-31.3
7			46.4	-41.7
-7			29.4	24.6
-11			30.7	-29.2
1	2	5	44.5	44.6
-3			29.4	-29.1
5			63.5	-57.1
7			29.4	23.7
-7			44.5	40.8
-9			32.7	-27.9
-3	2	7	28.1	-29.9
5			43.1	-40.2
-5			32.7	32.2
-7			47.8	47.2
-9			31.4	-30.5
-1	2	9	18.3	-23.5
-3			45.2	-45.3
-5			49.1	46.6
-1	2	11	30.7	-32.0
-9			25.5	17.9
-5	2	13	24.2	-22.7
0	3	1	25.9	-30.0
4			29.3	27.6
6			40.2	-38.1
-6			39.6	-38.2
2	3	3	33.4	-32.6
0			13.6	-15.9
-2			58.7	67.9
4			19.8	17.3
-4			14.3	-13.4
-12			26.6	-20.1
0	3	5	23.2	18.4
2			57.3	-53.8
6			29.9	28.8
-8			30.6	28.4
0	3	7	13.0	12.4
-4			38.2	-34.7
6			32.7	31.7
0	3	9	27.2	24.8
-2			25.9	-25.5
-6			26.6	20.2
-2	3	11	23.2	-21.1
-4			23.2	24.8
0	3	13	17.7	-21.3
-8			32.7	-29.2
0	3	15	10.2	-14.5
1	3	0	71.6	67.5
3			27.2	31.8
5			122.9	-120.2
7			43.0	45.1
9			43.0	44.9
11			37.5	-39.7
15			24.5	22.8
17	3	0	11.6	-16.2
3	3	2	64.1	63.8
-3			55.3	64.1
5			55.3	-53.9
-5			38.2	40.1
7			15.0	-16.7
-7			52.5	-49.9
9			76.4	73.0
-11			45.0	43.2
-13			33.4	-33.2
15			22.5	25.2
1	3	4	63.4	-64.0
-1			34.1	-34.8
3			103.1	109.9
-3			82.6	89.0
7			72.3	-68.8
-7			36.2	-35.0
-9			62.8	68.3
13			42.3	-37.9
-13			47.0	-47.3
1	3	6	86.0	-85.7
-1			25.2	25.4
3			54.6	50.4
5			58.7	57.1
-5			80.5	-85.3
7			43.6	-43.3
-9			66.2	64.2
11			35.5	34.7
-11			27.2	-26.8
-13			24.5	-24.5
-15			30.6	29.1
-1	3	8	58.7	56.5
3			38.9	-37.6
5			60.7	62.0
-5			79.2	-81.3
-7			43.6	41.6
-9			29.3	28.9
-11			40.9	-41.2
-1	3	10	61.4	59.3
3			53.9	-52.7
-3			44.3	-40.7
-7			50.4	48.9
9			33.4	-33.1
-9			23.2	-22.2
-11			29.9	-28.1
-13			32.0	34.2
1	3	12	35.5	35.0
3			24.5	-23.8
-3			38.9	-38.4
-5			27.9	24.1
7			34.1	34.1
-7			32.7	31.7
-9			56.0	-54.0
-5	3	14	48.4	50.3
-1	3	16	36.2	-34.5
0	4	0	58.6	63.7
4			43.8	-46.0
6			93.9	91.9
10			62.5	-64.1
12			16.4	17.0
16			13.3	-14.6
0	4	2	21.8	22.7
2			30.5	31.7
4			50.1	-48.3
-4			23.4	-23.4
6			21.1	19.4
-6			86.8	94.5
8			61.0	55.0
-8			53.2	-52.7
10			49.3	-48.3
-12			22.6	29.5
0	4	4	9.4	2.2
2			75.1	74.8
-2			96.2	-111.7
4			20.3	-17.4
-4			71.2	78.5
6			43.8	-38.7
8			44.6	41.4
-8			50.9	-52.3
12			29.7	-28.8
14			26.5	24.5
0	4	6	65.7	-65.9
2			85.3	75.1
-4			88.4	90.9
6			57.9	-54.6
-6			35.2	-35.2
0	4	8	78.2	-78.0
-2			50.9	51.2

Table 4 (*cont.*)

h	k	l	Fo	Fc
4	4	8	60.2	52.9
6			30.5	-29.8
-6			26.5	-27.7
10			30.5	30.9
0	4	10	13.3	-16.4
2			51.6	-48.2
-2			30.5	31.1
4			48.5	44.7
8			30.5	-28.4
-8			28.1	32.1
0	4	12	15.6	18.3
2			28.1	-29.3
-8			31.2	29.4
0	4	14	18.8	22.1
-4			28.9	-24.0
0	4	16	10.9	12.6
3	4	1	27.3	26.2
5			39.9	-39.7
-5			20.3	22.4
7			21.8	18.9
-7			39.1	-41.8
9			24.2	17.0
-11			30.5	31.1
-1	4	3	42.2	-43.5
3			18.0	22.8
-3			67.2	68.3
7			22.6	-22.2
-7			43.8	-42.5
1	4	5	61.7	-61.5
-1			28.9	24.5
3			41.4	37.6
-3			47.7	48.5
7			24.2	-22.1
-7			37.5	-37.9
1	4	7	46.1	-43.3
-3			39.9	37.6
5			39.9	38.7
-5			35.2	-33.4
-1	4	9	23.4	22.2
5			26.5	30.7
0	5	1	54.2	55.3
4			42.0	-45.2
-4			16.9	-16.1
6			21.0	22.1
-6			37.3	33.2
8			25.8	17.7
10			25.0	-23.3
0	5	3	14.9	13.4
2			17.6	22.2
-2			39.3	-45.3
4			40.6	-42.2
-6			32.5	38.5
8			30.5	31.5
0	5	5	25.0	-22.9
2			35.9	37.9
-2			32.5	-34.4
-4			33.2	35.1
-6			24.4	26.1
8			23.0	22.0
0	5	7	29.8	-32.4
2			29.1	28.4
-4			22.3	28.6
6			26.4	-26.1
0	5	9	22.3	-22.6
4			30.5	27.3
-6			21.7	-24.0
-8	5	11	24.4	23.0
0	5	15	13.5	16.2
1	5	0	81.3	-80.2
5			48.8	51.7
7			25.8	-23.6
9			23.7	-25.4
11			25.0	28.9
3	5	2	60.3	-65.0
-3			27.8	-27.6
5	5	2	50.9	51.1
-5			29.8	-32.1
-7			47.5	47.4
9			38.0	-39.6
-11			23.7	-19.5
1	5	4	42.0	43.0
-1			20.3	20.5
3			63.1	-63.1
-3			59.6	-67.1
-5			22.3	22.7
7			47.5	45.4
9			23.7	-17.5
-9			27.8	-26.3
1	5	6	54.2	53.4
-1			27.8	-28.4
-3			23.0	-16.8
5			48.1	-46.8
-5			41.4	43.8
7			38.0	33.5
-9			25.0	-21.7
1	5	8	23.7	23.2
-1			41.4	-45.1
3			28.4	27.8
5			44.0	-40.3
-7			23.7	-23.9
-11			37.3	31.1
1	5	10	22.3	-22.5
3			38.0	39.6
-7			38.0	-40.6
-9			26.4	21.4
-3	5	12	33.2	28.8
0	6	0	40.9	-39.8
6			31.2	-29.9
8			9.6	9.5
10			27.2	26.4
12			16.8	-16.2
2	6	2	20.9	-20.6
4			25.6	26.9
-6			29.7	-29.7
-8			34.5	35.3
0	6	4	27.2	26.2
2			33.7	-33.8
-2			30.4	30.6
-4			44.9	-47.2
-8			32.9	34.2
0	6	6	42.5	39.9
4			24.9	-23.9
-4			41.7	-42.5
6			32.9	28.3
0	6	8	36.9	33.9
4			31.2	-32.3
-6			32.1	31.1
0	6	10	8.8	6.7
-2			26.4	-24.0
0	6	12	14.4	-17.2
-4			33.7	27.3
0	6	14	19.2	-21.5
0	6	16	17.6	-8.9
3	6	1	26.4	-27.1
-3			24.1	23.6
-5			25.6	-34.8
-7			23.2	21.1
9			26.4	-26.8
-1	6	3	29.7	34.5
3			23.2	-24.0
-3			18.4	-16.4
7			27.2	26.7
-7			28.9	36.2
-1	6	5	27.2	27.5
-3			44.2	-50.9
-5			25.6	20.7
1	6	7	44.2	41.7
3			24.9	-21.3
-1	6	9	29.7	-26.3
-7			27.2	-26.3
0	7	1	21.1	23.7
-6			27.9	-27.0
2	7	3	21.1	-20.2
-2			24.9	30.9
4			23.4	21.6
-6			24.1	-17.9
0	7	5	21.1	15.9
-4			24.1	-31.4
0	7	7	26.4	28.4
-4			23.4	-22.6
0	7	9	13.5	19.8
-2			24.9	-17.5
-6			28.7	25.5
5	7	0	23.4	-22.6
7			11.2	11.6
9			15.9	14.6
11			16.6	-17.1
-7	7	2	26.4	-24.8
-3	7	4	27.1	30.8
1	7	6	24.1	-21.7
-3			23.4	22.1
-5			24.9	-22.2
-5	7	8	24.9	-17.9
-7			29.4	25.9
-3	7	10	30.1	-26.4
0	8	0	29.4	26.5
		2	11.5	13.4
		4	9.4	-9.3
		6	7.1	-11.9
		12	4.0	10.6
0	9	1	13.5	18.9
		3	8.5	8.8
		7	7.6	-13.8

An anisotropic least-squares refinement was carried out with the Busing & Levy program. Temperature factors of the form

$$\exp\{-[B_{11}h^2+B_{22}k^2+B_{33}l^2+2B_{12}hk+2B_{13}hl+2B_{23}kl]\}$$

are assumed for each atom. The final R_1 value is 7·0%. The positional parameters from the last anisotropic least-squares refinement are listed in Table 2, the temperature factor coefficients in Table 3, and the observed and calculated structure factors in Table 4.

Table 5. *Interatomic distances with standard deviations from anisotropic least-squares refinement*

Model *A* corresponds to distances uncorrected for thermal motion. Models *B* and *C* correspond to interatomic distances averaged over thermal motion in which either the second atom is assumed to ride on the first (Model *B*) or the atoms are assumed to move independently (Model *C*). Standard deviations are virtually identical for each of the three calculated models (Busing & Levy, 1959)

Distance	Model *A* Value	Model *B* Value	Model *C* Value	σ
Mn–Mn	2·923 Å			0·003 Å
Mn–C_1	1·792	1·826 Å	1·874 Å	0·014
Mn–C_2	1·855	1·864	1·911	0·015
Mn–C_3	1·830	1·835	1·882	0·016
Mn–C_4	1·811	1·818	1·857	0·016
Mn–C_5	1·826	1·826	1·866	0·014
C_1–O_1	1·151	1·229	1·396	0·016
C_2–O_2	1·147	1·183	1·278	0·015
C_3–O_3	1·160	1·208	1·302	0·017
C_4–O_4	1·156	1·198	1·287	0·016
C_5–O_5	1·166	1·205	1·284	0·016

Table 6. *Bond angles with standard deviations from anisotropic least-squares refinement*

Angle	Value	σ
Mn–C_1–O_1	177·0°	1·6°
Mn–C_2–O_2	178·2	1·1
Mn–C_3–O_3	177·8	1·3
Mn–C_4–O_4	175·5	1·2
Mn–C_5–O_5	177·8	1·3
C_1–Mn–C_2	96·1	0·6
C_1–Mn–C_3	93·8	0·6
C_1–Mn–C_4	93·0	0·7
C_1–Mn–C_5	92·3	0·7
C_2–Mn–C_3	170·1	0·5
C_2–Mn–C_4	88·9	0·6
C_2–Mn–C_5	88·9	0·6
C_3–Mn–C_4	89·7	0·6
C_3–Mn–C_5	91·6	0·6
C_4–Mn–C_5	174·5	0·6
C_1–Mn–Mn′	177·3	0·5
C_2–Mn–Mn′	85·5	0·4
C_3–Mn–Mn′	84·6	0·4
C_4–Mn–Mn′	89·2	0·4
C_5–Mn–Mn′	85·7	0·4

Interatomic distances and bond angles and their standard deviations were calculated with the Busing & Levy (1959) Function and Error Program. The intramolecular distances for the anisotropic refinement are given in Table 5 and the bond angles in Table 6. Although the changes in positional parameters brought about by the inclusion of anisotropic temperature factors are within three standard deviations (the greatest shift of almost 3σ was for the *y* parameter of O_1), the Mn–C_1–O_1 bond angle changed over three standard deviations and the bond lengths and angles showed greater internal consistency. As expected, the standard deviations are lower for the anisotropic refinement. It is felt that the positional parameters for the anisotropic analysis are probably more reliable, since the model is more realistic.

Analysis of anisotropic thermal motion

A qualitative indication of the thermal anisotropy of atoms in the molecular crystal of $Mn_2(CO)_{10}$ can

Table 7. *The principal axes, r.m.s. thermal displacements and orientations with crystallographic axes*

Atom	r	$\mu(r)$	$\varphi(r, a)$	$\varphi(r, b)$	$\varphi(r, c)$
Mn	1	0·161 ± 0·008 Å	91·7 ± 4·7°	138·6 ± 4·9°	49·8 ± 3·9°
	2	0·192 ± 0·002	155·5 ± 3·1	104·6 ± 3·5	94·7 ± 5·5
	3	0·243 ± 0·004	114·4 ± 2·8	52·3 ± 3·8	40·6 ± 3·3
C_1	1	0·215 ± 0·015	42·4 ± 8·4	91·2 ± 15·7	62·6 ± 8·0
	2	0·274 ± 0·020	109·6 ± 15·6	151·5 ± 12·9	65·5 ± 13·7
	3	0·342 ± 0·020	125·8 ± 7·6	61·5 ± 12·9	38·3 ± 9·8
O_1	1	0·223 ± 0·014	46·1 ± 3·1	93·0 ± 5·0	59·1 ± 2·9
	2	0·391 ± 0·017	64·3 ± 7·5	34·2 ± 9·4	117·3 ± 7·9
	3	0·476 ± 0·019	125·1 ± 5·7	55·9 ± 9·4	43·6 ± 6·5
C_2	1	0·169 ± 0·017	44·0 ± 8·6	108·6 ± 7·2	65·8 ± 7·9
	2	0·257 ± 0·019	46·3 ± 9·2	64·6 ± 31·4	137·9 ± 27·1
	3	0·282 ± 0·019	94·5 ± 23·4	32·3 ± 27·3	57·9 ± 29·6
O_2	1	0·165 ± 0·017	127·6 ± 4·9	118·9 ± 3·6	40·1 ± 4·5
	2	0·280 ± 0·012	139·4 ± 5·8	82·5 ± 7·5	114·8 ± 6·4
	3	0·347 ± 0·014	103·1 ± 6·8	30·0 ± 4·2	60·7 ± 5·2
C_3	1	0·182 ± 0·018	73·5 ± 7·7	75·7 ± 10·0	34·8 ± 8·2
	2	0·265 ± 0·019	78·5 ± 41·8	163·8 ± 23·3	82·1 ± 24·0
	3	0·286 ± 0·017	20·3 ± 25·3	82·6 ± 41·8	123·6 ± 10·1
O_3	1	0·185 ± 0·016	123·3 ± 3·3	117·4 ± 6·3	35·3 ± 6·6
	2	0·282 ± 0·015	96·4 ± 7·0	141·9 ± 6·6	123·8 ± 6·7
	3	0·373 ± 0·014	34·1 ± 3·6	114·3 ± 6·2	81·2 ± 4·5
C_4	1	0·191 ± 0·017	4·9 ± 16·7	89·2 ± 17·8	109·9 ± 14·7
	2	0·230 ± 0·019	93·6 ± 21·8	37·1 ± 14·4	124·3 ± 14·4
	3	0·288 ± 0·018	86·6 ± 9·3	52·9 ± 14·3	41·2 ± 13·0
O_4	1	0·204 ± 0·017	54·2 ± 6·0	142·9 ± 7·3	107·0 ± 8·0
	2	0·279 ± 0·014	62·2 ± 8·8	61·4 ± 8·4	147·1 ± 8·1
	3	0·353 ± 0·014	48·4 ± 6·0	68·5 ± 5·7	62·8 ± 7·8
C_5	1	0·175 ± 0·017	82·9 ± 18·7	107·5 ± 46·3	28·1 ± 16·6
	2	0·194 ± 0·023	110·9 ± 12·2	154·5 ± 34·9	98·0 ± 43·7
	3	0·283 ± 0·018	22·2 ± 9·9	107·9 ± 10·6	116·8 ± 7·6
O_5	1	0·223 ± 0·014	74·5 ± 5·2	59·8 ± 23·9	43·5 ± 16·1
	2	0·250 ± 0·015	95·5 ± 9·0	30·3 ± 23·8	117·0 ± 19·6
	3	0·351 ± 0·014	16·5 ± 4·7	93·0 ± 6·0	121·1 ± 4·9

Table 8. *R.M.S. components of thermal displacements with standard deviations for oxygen atoms*

Atom	Along Mn–C bond direction $u(1)$	Perpendicular to Mn–C bond direction $u(2)$
O_1	0·225 ± 0·014 Å	0·419 ± 0·018 Å
O_2	0·170 ± 0·017	0·282 ± 0·012
O_3	0·191 ± 0·016	0·354 ± 0·013
O_4	0·230 ± 0·016	0·337 ± 0·013
O_5	0·262 ± 0·015	0·270 ± 0·012

be obtained by analysis of the B_{ij} coefficients. The three principal (orthogonal) axes of the ellipsoid describing the anisotropic temperature factor were computed for each atom (Busing & Levy, 1958). Table 7 gives $\mu(r)$, the calculated r.m.s. component of thermal displacement of the atom along the rth principal axis ($r=1$, 2, or 3); and $\varphi(r, i)$, the angles made by the rth principal axis with the ith crystallographic axis. The degree of anisotropy of each of the atoms is inferred from the differences in magnitude of the r.m.s. thermal displacements along the three principal axes. In order to indicate the thermal motions of the individual carbonyl groups with respect to the molecule, the calculated r.m.s. components of thermal displacement of the oxygen atoms both parallel and perpendicular to the Mn–C bond directions are given in Table 8. In general, the displacements of the oxygen atoms normal to the Mn–C bond directions are greater than the displacements along the Mn–C bonds. As expected, the largest observed difference occurs for the O_1 atom of the apical carbonyl group. Qualitative agreement was found between these results and the thermal anisotropies indicated on the isotropic $(F_o - F_c)$ syntheses.

The calculated mean r.m.s. radial thermal displacements of the atoms are listed in Table 9. The radial displacement values are 0·49 Å for C_1 and 0·65 Å for O_1, whereas for the other four carbonyl groups the average carbon and oxygen radial displacements are 0·41 Å and 0·49 Å, respectively.

Because of the possible accumulation of systematic errors in the anisotropic temperature factors, it is difficult to attach *definite* physical significance to the calculated amplitudes of thermal vibration, and the results at most are qualitative.

Two models (*B* and *C*) were utilized for calculating intramolecular bond distances averaged over thermal motion. In the first model (*B*) the second atom is

Table 9. *Mean r.m.s. radial thermal displacements with standard deviations*

Atom	Radial thermal displacements
Mn	0·349 ± 0·006 Å
C_1	0·488 ± 0·014
O_1	0·655 ± 0·014
C_2	0·417 ± 0·014
O_2	0·476 ± 0·011
C_3	0·430 ± 0·014
O_3	0·504 ± 0·011
C_4	0·416 ± 0·013
O_4	0·494 ± 0·011
C_5	0·385 ± 0·014
O_5	0·485 ± 0·011

assumed to ride on the first, while in the second model (*C*) the atoms are assumed to move independently (Busing & Levy, 1959). For comparison these values are listed in Table 5 adjacent to the thermally uncorrected anisotropic bond lengths (model *A*). For model *B* the increase in length of the Mn–C_1 distance is $2 \cdot 4\sigma$, whereas for the other four Mn–C distances the increases are less than 1σ. The increase in the apical C_1–O_1 distance is 5σ while the increases in the other C–O distances are 2–3σ. For model C the increases in the Mn–C_1 distance and the other four Mn–C distances are 6σ and 3–4σ, respectively. The corresponding increases in the C_1–O_1 distance and the other four C–O distances are 15σ and 7–9σ, respectively. Although the bond length changes in general are large, neither of these thermal models (*B* or *C*) is felt to conform to the actual physical situation present in $Mn_2(CO)_{10}$, and the preferred values are those with no thermal correction. The bonded atoms certainly do not move completely independently and the 'piggy-back model' is not applicable for the lighter carbonyl atoms.

Discussion

Dimanganese decacarbonyl consists of discrete molecules of approximate point group symmetry D_{4d}. Each manganese atom is octahedrally coordinated to five carbonyl groups and the other manganese atom in such a way that the equatorial carbonyl groups are arranged in a staggered configuration. Fig. 1 shows the molecular configuration with the intramolecular bond lengths and angles calculated from the anisotropic least-squares refinement without correction for thermal motion. The two halves of the dimeric molecule are symmetrically related by a two-fold axis which is required by the space group $I2/a$. The mean uncorrected length of the four equatorial Mn–C bonds is 1·83 Å compared with the uncorrected apical Mn–C length of 1·79 Å. The mean uncorrected C–O distance of 1·16 Å is in good agreement with carbonyl distances for other metal carbonyls. The fact that the calculated thermal corrections for models *B* and *C* (Table 5) are so large makes it difficult to give real meaning to small differences in bond angles and distances in $Mn_2(CO)_{10}$.

The intramolecular non-bonding distances are given in Fig. 2. The average minimum intramolecular C · · · C distances are 2·6 Å within the same half of the dimer

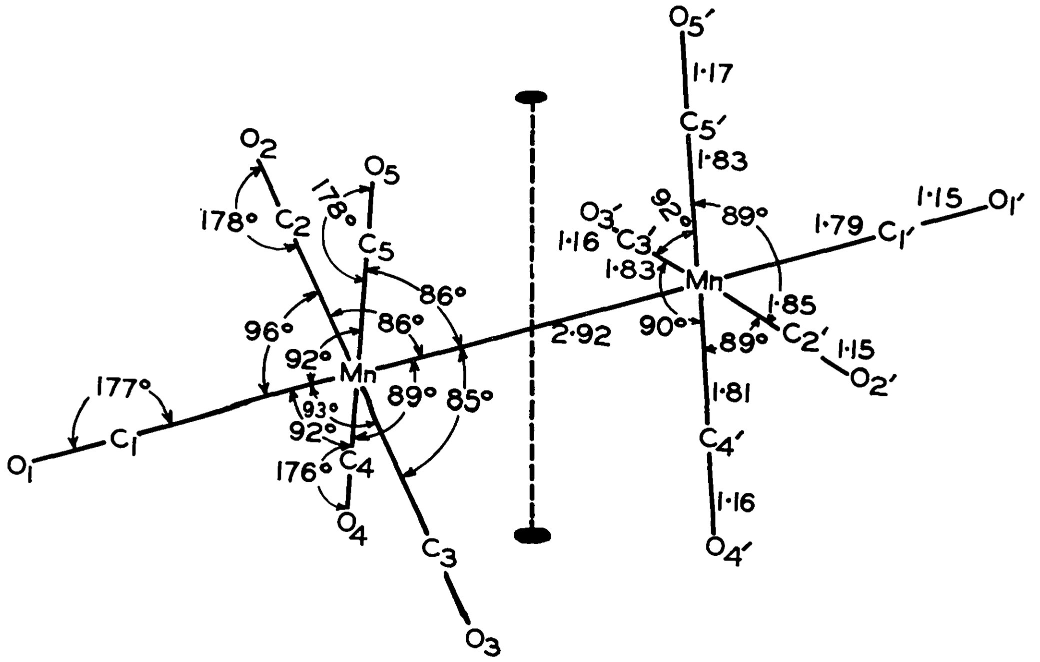

Fig. 1. The molecular configuration of $Mn_2(CO)_{10}$ with final bond distances and angles uncorrected for thermal motion. The two halves of the dimeric molecule are symmetrically related by the indicated crystallographic 2-fold axis.

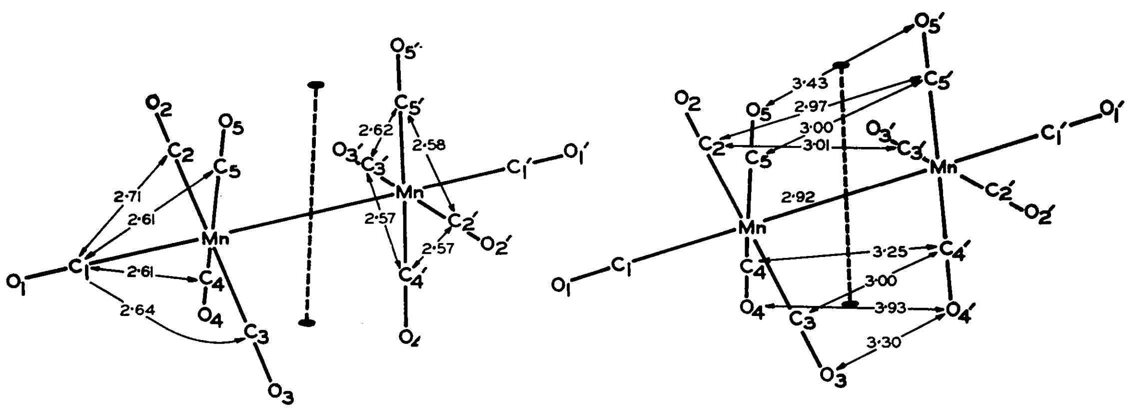

Fig. 2. Non-bonding intramolecular interactions in $Mn_2(CO)_{10}$.

and 3·0 Å between the two halves of the dimer. The average minimum intramolecular C · · · O distances are 3·5 Å within the same half of the dimer and 3·3 Å between the two halves of the dimer. Minimum intermolecular van der Waals distances are 3·05 Å for O · · · O contacts and 3·2 Å for C · · · O contacts.

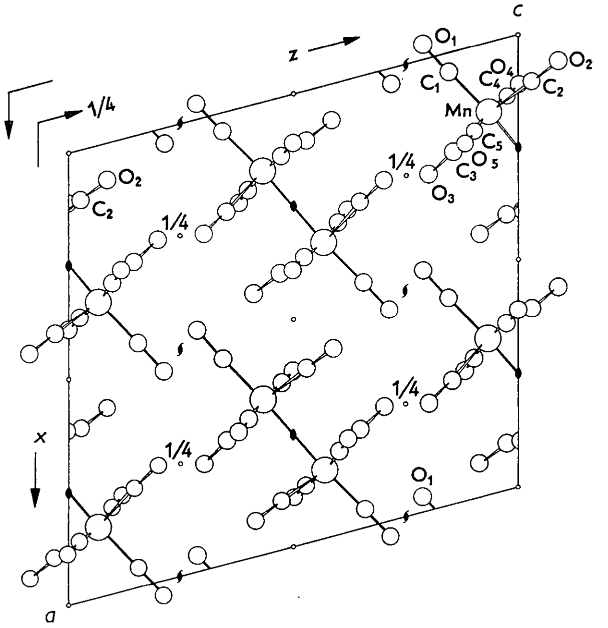

Fig. 3. [010] projection of the unit cell.

The arrangement of the molecules in the unit cell viewed down [010] is shown in Fig. 3. The Mn–Mn directions in the dimeric molecules are required by crystallographic symmetry to be parallel to one another. The four pairs of manganese atoms lie in four planes perpendicular to *b* at fractional *y* values of 0·230, 0·270, 0·730, and 0·770. The angles between the Mn–Mn molecular bond axis and the crystallographic *a* and *c* axes are 42° and 63°, respectively. If strict D_{4d} molecular symmetry is assumed, the orientation of the molecules in the unit cell is also limited by the crystallographic 2-fold axis which bisects the molecule. The Mn–CO angle of tilt from the plane which contains two dimeric manganese atoms would be 22·5° for two of the four ligands on each manganese atom (*i.e.*, one ligand would be tipped upward 22·5° and the other one tilted downward 22·5°). The other two CO's would then be at an angle of 67·5° with respect to the same plane.

The molecule is found to be somewhat distorted from the idealized D_{4d} configuration. The four equatorial Mn–CO bonds are bent inward toward the other half of the molecule (see Fig. 1) so that the manganese atom is 0·12 Å out of the mean least-squares plane containing C_2, C_3, C_4, and C_5. It might be expected that equatorial carbonyl–carbonyl repulsions would bend the equatorial groups outward, but the non-bonding intramolecular distances shown in Fig. 2 indicate that the apical, equatorial C · · · C repulsions in one half of the molecule are stronger than the equatorial, equatorial C · · · C repulsions between the two halves of the molecule. Although such intramolecular repulsions are probably the main factor in determining the inward bending of the equatorial CO's, part of this distortion may be the influence of neighboring molecules, since the distortion also increases the intermolecular O · · · O distances.

The $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$ compounds were the first polynuclear metal carbonyls known to be held together only by direct metal–metal bonds. These and the isomorphous compounds $(C_5H_5W)_2(CO)_6$ and $(C_5H_5Mo)_2(CO)_6$ (Wilson & Shoemaker, 1957) were the first well-established examples of dimeric transition metal complexes with metal–metal bonds alone linking the dimer. The metal–metal bond in each of the four compounds enables each transition metal to attain a 'closed-shell' electronic configuration, in accord with the compound's observed diamagnetism.

The refined Mn–Mn distance of 2·923 Å is approximately 0·5 Å longer than the Mn–Mn distance obtained from the sum of 'normal' covalent radii. This large difference probably can be attributed mainly to the negative charge localized on the metal atom through coordination with the CO ligands. Of course, some delocalization of charge may be obtained by utilization of the *d*-orbital electrons of the metal in π-bonding with the empty antibonding MO's of the ligands. The strength of the Mn–Mn bond has been estimated as 34 ± 13 kcal.mol^{-1} (Cotton & Monchamp, 1960).

$Tc_2(CO)_{10}$ (Hileman *et al.*, 1961) has been shown (Trueblood & Wallach, 1961) to be isomorphous with $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$. A three-dimensional X-ray examination of $Tc_2(CO)_{10}$ is in progress (Fisher & Dahl, to be published) for the purpose of comparing its molecular features with those of the manganese and rhenium compounds. Other recently prepared isoelectronic dimeric species with presumably similar molecular configurations include

$$[Cr_2(CO)_{10}]^{2-},\ [Mo_2(CO)_{10}]^{2-},\ [W_2(CO)_{10}]^{2-},\ [Co_2(CN)_{10}]^{6-},\ \text{and}\ [Co_2(CNCH_3)_{10}]^{4+}.$$

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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A refinement of the crystal structure of sanidinized orthoclase.

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Introduction

The structure of sanidine, a monoclinic potash felspar, was first examined by Taylor (1933). In 1949 Cole, Sörum & Kennard published a full three-dimensional refinement of this structure, calling it 'sanidinized orthoclase' because the crystal they examined was orthoclase (Spencer's (1937) specimen 'C') irreversibly inverted to the form of natural sanidine by extended heat-treatment at 1000°C. Their paper contains details of the physical and chemical properties of this material. Because the hand-calculated atomic coordinates which they report for sanidine gave an R-factor $\Sigma||F_o|-|F_c||/\Sigma|F_o| = 0{\cdot}14$, it was thought worth while to press the refinement somewhat further, using their photometrically measured structure factors (Cole, 1949) and an automatic three-dimensional refinement program.

The need to know this structure with the maximum attainable accuracy arises from recent rapid advances in the knowledge of other felspar structures, notably those of celsian, microcline, maximum microcline, low albite, high albite, bytownite, primitive anorthite and