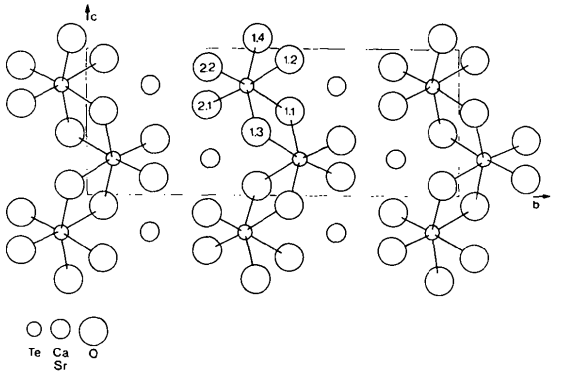

Fig. 1. The structure projected along **a**.

Discussion. The structure of these compounds is given in Fig. 1. It exhibits octahedrally coordinated Te atoms in infinite chains along **c**, similar to those in Na_2TeO_4 (Kratochvil & Jensovsky, 1977).

The Ca and Sr atoms are also octahedrally coordinated by O atoms with Ca—O ranging from 2·34 (3) to 2·39 (4) Å and Sr—O from 2·47 (3) to 2·61 (4) Å.

The authors thank Mr P. van Vlaanderen of ECN, Petten, for providing the step-scanned X-ray data.

References

BAGLIO, J. A. & NATANSOHN, S. (1969). *J. Appl. Cryst.* **2**, 252–254.

KRATOCHVIL, B. & JENSOVSKY, L. (1977). *Acta Cryst.* B**33**, 2596–2598.

RUTTEN-KEULEMANS, E. W. M. (1973). Private communication.

SLEIGHT, A. W., FORIS, C. M. & LICIS, M. S. (1972). *Inorg. Chem.* **11**, 1157–1158.

TRÖMEL, M. (1972). *J. Appl. Cryst.* **5**, 241–242.

Acta Cryst. (1979). B**35**, 729–730

Bis{μ-[bromo(pentacarbonylmanganio)germanium(IV)]}-octacarbonyldimanganese

BY HANS PREUT AND HANS-JÜRGEN HAUPT

Lehrstuhl für Anorganische Chemie II *der Universität, Postfach* 500500, *D*-4600 *Dortmund* 50, *Federal Republic of Germany*

(*Received* 26 *October* 1978; *accepted* 30 *November* 1978)

Abstract. $Ge_2Mn_4Br_2(CO)_{18}$, M_r = 1028·94, monoclinic, $P2_1/c$, a = 8·762 (4), b = 12·124 (4), c = 15·425 (4) Å, β = 62·82 (9)°, U = 1458 Å^3, Z = 2, D_c = 2·343 Mg m^{-3}; $F(000)$ = 972; Mo $K\alpha$ radiation, λ = 0·71069 Å, μ(Mo $K\alpha$) = 6·37 mm^{-1}. The structure was refined to an R of 0·0325 for 1397 unique diffractometer data. The central fragment of the molecule consists of a planar Mn_2Ge_2 rhombus with a Mn—Mn bond [r(Mn—Mn) = 2·923 (2) Å] across the metal ring.

Introduction. We have recently reported the structures of $Mn_2(CO)_8[\mu\text{-Sn(Br)Mn(CO)}_5]_2$ (Preut & Haupt, 1976) and $Mn_2(CO)_8[\mu\text{-Sn(Cl)Mn(CO)}_5]_2$ (Haupt, Preut & Wolfes, 1978). As part of our study of compounds with a covalent metal–metal bond we have determined the crystal structure of $Mn_2(CO)_8[\mu\text{-Ge(Br)Mn(CO)}_5]_2$. The crystal was prepared with the starting materials $Br_3GeMn(CO)_5$ and $BrMn(CO)_5$ (Ködel, Haupt & Huber, 1979).

Three-dimensional intensity data were collected using a crystal of dimensions 0·18 [100] × 0·07 [010] × 0·09 [001] mm. Unit-cell parameters were determined by least-squares fits to the reflecting positions of 23 reflections on a Hilger & Watts Y 290 automatic four-circle diffractometer with graphite-monochromatized Mo $K\alpha$ radiation and a scintillation counter. The intensities of 1543 reflections ($I > 3\sigma$) with $2° \le \theta \le 24·3°$ were measured by the $\omega/2\theta$ scan technique, with a scan width $\Delta 2\theta$ = (1·34 + 0·34 tan θ)° from background to background and a scan speed of 0·02° s^{-1} in 2θ. Backgrounds were measured at each end of the scan range for a time of 7 s. Four standard reflections were measured after every fifty reflections during the data collection and showed only random deviations from their mean intensities. Lorentz and polarization corrections (but no correction for absorption) were applied and after the equivalent reflections were averaged the data set contained 1397 unique reflections for the structure analysis. The structure was solved by Patterson and Fourier methods and refined by a least-squares method (unit weights) with *SHELX* (Sheldrick, 1976). The refinement con-

0567-7408/79/030729-02$01.00

verged to $R = \sum \Delta / \sum F_o = 0.0325$ for 199 refined parameters.

Atomic scattering factors have been taken from Cromer & Mann (1968) and Cromer & Liberman (1970).

Positional parameters are given in Table 1, bond lengths and angles in Table 2.* Fig. 1 shows the molecule with the atom-numbering scheme.

Discussion. $Mn_2(CO)_8[\mu\text{-Ge(Br)Mn(CO)}_5]_2$ is isotypic with the compounds $Mn_2(CO)_8[\mu\text{-Sn}(X)\text{Mn(CO)}_5]_2$ (X = Cl, Br) (Preut & Haupt, 1976; Haupt, Preut & Wolfes, 1978).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34121 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final positional parameters* ($\times 10^4$) *with standard deviations in parentheses*

	x	y	z
Ge(1)	612 (1)	3398 (1)	4758 (1)
Br(1)	−1745 (1)	2243 (1)	4916 (1)
Mn(1)	−501 (2)	4844 (1)	6035 (1)
Mn(2)	2989 (2)	2026 (1)	4303 (1)
C(1)	4666 (14)	980 (10)	4021 (8)
C(2)	3566 (12)	2682 (9)	5212 (8)
C(3)	1369 (14)	1165 (8)	5289 (7)
C(4)	2311 (13)	1441 (8)	3399 (7)
C(5)	4516 (14)	2919 (9)	3313 (7)
C(6)	1705 (12)	5178 (9)	5852 (7)
C(7)	−2721 (12)	4554 (8)	6258 (6)
C(8)	−658 (12)	3633 (8)	6769 (6)
C(9)	−1289 (12)	5796 (8)	7041 (6)
O(1)	5667 (13)	324 (8)	3866 (7)
O(2)	3885 (9)	3044 (7)	5775 (5)
O(3)	415 (12)	626 (7)	5889 (6)
O(4)	1931 (10)	1073 (7)	2860 (6)
O(5)	5441 (11)	3444 (7)	2692 (6)
O(6)	3003 (9)	5365 (7)	5791 (6)
O(7)	−4113 (9)	4369 (7)	6474 (6)
O(8)	−829 (10)	2910 (6)	7264 (5)
O(9)	−1821 (10)	6368 (6)	7692 (5)

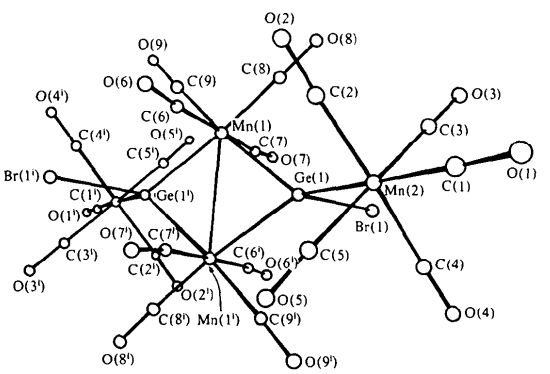

Fig. 1. Drawing of the molecule $Mn_2(CO)_8[\mu\text{-Ge(Br)Mn(CO)}_5]_2$ and the atom-numbering scheme. Symmetry code (i) $\bar{x}$, $1-y$, $1-z$.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

Ge(1)–Br(1)	2·413 (1)	Mn(1)–Ge(1)–Mn(1ⁱ)	72·20 (5)
Ge(1)–Mn(1)	2·480 (2)	Ge(1)–Mn(1)–Ge(1ⁱ)	107·80 (6)
Ge(1)–Mn(2)	2·502 (2)	Mn(1)–Ge(1)–Mn(2)	131·88 (7)
Ge(1)–Mn(1ⁱ)	2·482 (2)	Mn(1ⁱ)–Ge(1)–Mn(2)	130·36 (6)
Mn(1)–Mn(1ⁱ)	2·923 (2)	Mn(1)–Ge(1)–Br(1)	108·78 (6)
Mn(1)–C(6)	1·866 (10)	Mn(1ⁱ)–Ge(1)–Br(1)	108·91 (6)
Mn(1)–C(7)	1·848 (10)	Mn(2)–Ge(1)–Br(1)	101·95 (6)
Mn(1)–C(8)	1·820 (10)	Ge(1)–Mn(1)–C(6)	91·6 (3)
Mn(1)–C(9)	1·800 (10)	Ge(1)–Mn(1)–C(7)	90·7 (3)
Mn(2)–C(1)	1·837 (11)	Ge(1)–Mn(1)–C(8)	79·3 (3)
Mn(2)–C(2)	1·872 (12)	Ge(1)–Mn(1)–C(9)	174·4 (3)
Mn(2)–C(3)	1·857 (11)	Ge(1ⁱ)–Mn(1)–C(6)	90·6 (3)
Mn(2)–C(4)	1·886 (11)	Ge(1ⁱ)–Mn(1)–C(7)	88·9 (3)
Mn(2)–C(5)	1·852 (12)	Ge(1ⁱ)–Mn(1)–C(8)	172·1 (3)
C(1)–O(1)	1·125 (12)	Ge(1ⁱ)–Mn(1)–C(9)	77·8 (3)
C(2)–O(2)	1·117 (12)	Ge(1)–Mn(2)–C(2)	89·0 (4)
C(3)–O(3)	1·129 (11)	Ge(1)–Mn(2)–C(3)	85·2 (3)
C(4)–O(4)	1·119 (11)	Ge(1)–Mn(2)–C(4)	87·4 (3)
C(5)–O(5)	1·127 (12)	Ge(1)–Mn(2)–C(5)	92·2 (4)
C(6)–O(6)	1·121 (11)	C(1)–Mn(2)–C(2)	90·6 (5)
C(7)–O(7)	1·131 (10)	C(1)–Mn(2)–C(3)	92·0 (5)
C(8)–O(8)	1·127 (11)	C(1)–Mn(2)–C(4)	93·1 (5)
C(9)–O(9)	1·131 (10)	C(1)–Mn(2)–C(5)	90·6 (5)
		C(2)–Mn(2)–C(3)	89·6 (5)
		C(2)–Mn(2)–C(5)	91·7 (5)
		C(3)–Mn(2)–C(4)	90·8 (4)
		C(4)–Mn(2)–C(5)	87·9 (4)
		C(6)–Mn(1)–C(7)	177·7 (4)
		C(6)–Mn(1)–C(9)	87·4 (4)
		C(7)–Mn(1)–C(8)	87·5 (4)
		C(7)–Mn(1)–C(9)	90·3 (4)
		C(8)–Mn(1)–C(9)	95·2 (4)

Symmetry code: (i) $\bar{x}$, $1-y$, $1-z$.

The central structural element of these molecules is the planar metal ring M_2Mn_2 (M = Ge, Sn). The M–Mn–M angles [X = Br, M = Ge: 72·20 (5); X = Cl, M = Sn: 72·17 (2); X = Br, M = Sn: 71·91 (2)°] are characteristic of Ge^{IV} and Sn^{IV} (approximately 72°), while they are significantly greater [M = Ga: 76·86 (2); M = In: 76·36 (2)°] in the compounds $Mn_2(CO)_8[\mu\text{-}M\text{Mn(CO)}_5]_2$ (M = Ga, In) (Preut & Haupt, 1974), which have similar flat metal rings. The values of these angles are in all these cases an indication that there is a bond between opposite Mn atoms across the ring. This Mn–Mn distance decreases with the size of the bridging atom in the compounds mentioned above.

References

Cromer, D. T. & Liberman, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

Haupt, H.-J., Preut, H. & Wolfes, W. (1978). *Z. Anorg. Allg. Chem.* **446**, 105–118.

Ködel, W., Haupt, H.-J. & Huber, F. (1979). *Z. Anorg. Allg. Chem.* In the press.

Preut, H. & Haupt, H.-J. (1974). *Chem. Ber.* **107**, 2860–2869.

Preut, H. & Haupt, H.-J. (1976). *Z. Anorg. Allg. Chem.* **422**, 47–53.

Sheldrick, G. M. (1976). Personal communication.