Bromopentacarbonylmanganese

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Key indicators

Single-crystal X-ray study

$T = 100$ K

Mean σ(O–C) = 0.005 Å

R factor = 0.032

wR factor = 0.076

Data-to-parameter ratio = 15.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The Mn and Br atoms as well as one of the carbonyl groups of the title compound, [MnBr(CO)$_5$], are located on a crystallographic mirror plane. As a result, there is just half a molecule in the asymmetric unit displaying C_s symmetry. However, the deviations from C_{4v} symmetry are very small. BrMn(CO)$_5$ is isomorphous with ClMn(CO)$_5$ and CH$_3$Mn(CO)$_5$.

Comment

The central Mn atom in BrMn(CO)$_5$ is octahedrally coordinated. The molecule has C_s symmetry. Mn, Br and one of the carbonyl groups are located on a mirror plane perpendicular to the b axis. The deviations from C_{4v} symmetry are very small. The Mn—C bond *trans* to the Mn—Br bond is significantly shorter than the equatorial Mn—C bonds. BrMn(CO)$_5$ is isomorphous with ClMn(CO)$_5$ (Greene & Bryan, 1971) and CH$_3$Mn(CO)$_5$ (Andrews *et al.*, 1983). Unfortunately, the methyl group in the latter structure is statistically disordered over all six coordination sites about the Mn atom.

Experimental

BrMn(CO)$_5$ was dissolved in C$_6$D$_6$ and heated to 353 K for 24 h. When the solution was cooled to room temperature, BrMn(CO)$_5$ precipitated as yellow crystals.

Crystal data

[MnBr(CO)$_5$]	Mo $K\alpha$ radiation
$M_r = 274.90$	Cell parameters from 11620
Orthorhombic, $Pnma$	reflections
$a = 11.6252\ (16)$ Å	$\theta = 3.8–27.6°$
$b = 11.3317\ (18)$ Å	$\mu = 6.66$ mm^{-1}
$c = 6.0403\ (10)$ Å	$T = 100\ (2)$ K
$V = 795.7\ (2)$ Å^3	Prism, yellow
$Z = 4$	$0.22 \times 0.14 \times 0.12$ mm
$D_x = 2.295$ Mg m^{-3}	

Data collection

Stoe IPDS-II two-circle diffractometer	958 independent reflections
ω scans	772 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)	$R_{int} = 0.074$
	$\theta_{max} = 27.6°$
	$h = -14 \rightarrow 15$
$T_{min} = 0.290$, $T_{max} = 0.452$	$k = -14 \rightarrow 14$
9213 measured reflections	$l = -7 \rightarrow 7$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o{}^2) + (0.0409P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o{}^2 + 2F_c{}^2)/3$
$wR(F^2) = 0.076$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
958 reflections	$\Delta\rho_{min} = -1.25$ e Å^{-3}
61 parameters	

Table 1
Selected geometric parameters (Å, °).

|			
Mn1—C1	1.821 (6)	O1—C1	1.149 (7)
Mn1—C2	1.889 (4)	O2—C2	1.134 (4)
Mn1—C3	1.892 (4)	O3—C3	1.132 (4)
Mn1—Br1	2.5158 (10)		
C1—Mn1—C2	92.41 (16)	C2—Mn1—Br1	87.51 (11)
C2^i—Mn1—C2	89.3 (2)	C3—Mn1—Br1	88.16 (11)
C2—Mn1—C3^i	175.46 (16)	O1—C1—Mn1	179.0 (5)
C1—Mn1—C3	91.93 (16)	O2—C2—Mn1	178.1 (3)
C2—Mn1—C3	89.16 (14)	O3—C3—Mn1	177.2 (3)
C1—Mn1—Br1	179.88 (17)		

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

The deepest hole in the difference electron density map is located 0.83 Å from Br1.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

References

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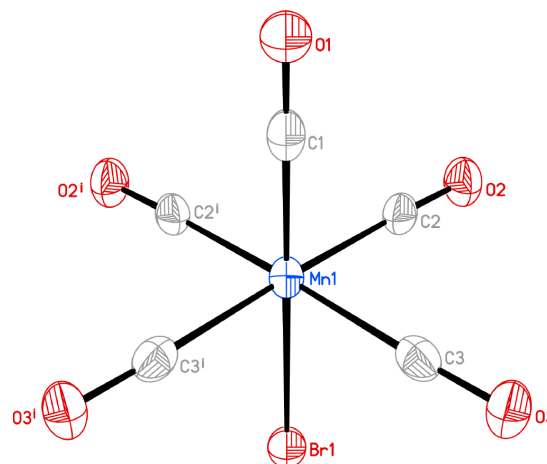
Figure 1
Perspective view of the title compound, with the atom-numbering scheme; displacement ellipsoids are at the 50% probability level. The symmetry operator for generating equivalent atoms is (i) $x, \frac{1}{2} - y, z$.

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