Journal of Organometallic Chemistry
Elsevier Sequoia S.A., Lausanne
Printed in The Netherlands

MOLECULAR STRUCTURE OF (TRIBROMOGERMYL)MANGANESE PENTACARBONYL, $Br_3GeMn(CO)_5$

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(Received February 15th, 1970))

SUMMARY

The molecular structure of $Br_3GeMn(CO)_5$ was determined by electron diffraction and the following bond lengths were found: Mn–Ge 2.44, Ge–Br 2.31, Mn–C 1.84, C–O 1.16 Å.

INTRODUCTION

The synthesis and properties of (tribromogermyl)manganese pentacarbonyl, $Br_3GeMn(CO)_5$, have been reported previously[1,2]. In this communication we wish to present the results of the electron diffraction study of this compound in the vapour phase.

RESULTS AND DISCUSSION

The electron diffraction patterns were recorded on a EG-100M electronograph with the r^3-sector. The nozzle-to-plate distances were ca. 400 mm and 200 mm and accelerating potential of 40 kV was used. The modified molecular intensity function $s \cdot M(s)$ calculated in the usual way[3-5], covers the s range from 1.3 to 27.6 $Å^{-1}$.

The molecular structure was determined by radial distribution method with the following assumptions: all the Mn–C–O fragments are linear, the angles at the Mn atom are octahedral and at the Ge atom tetrahedral. The structure was refined by least squares procedure in a version of stage-by-stage parameter refinement applied to the radial distribution and the molecular intensity curves.

For this purpose we used the program of the theoretical $s \cdot M(s)$ curve calculation taking into account non-nuclear scattering[6]. Hartree–Fock potentials[7] for Mn, C and O atoms and Thomas–Fermi–Dirac potentials[8] for Ge and Br atoms were used. The function of non-coherent electron scattering, $S(s)$, was taken from Tietz's equation[9]; the phase shift $\Delta\eta$ was calculated using the reported method[10].

The molecular geometry of $Br_3GeMn(CO)_5$ and the main parameters are given in Fig. 1.

The Ge atom co-ordination is distorted tetrahedral with following angles:

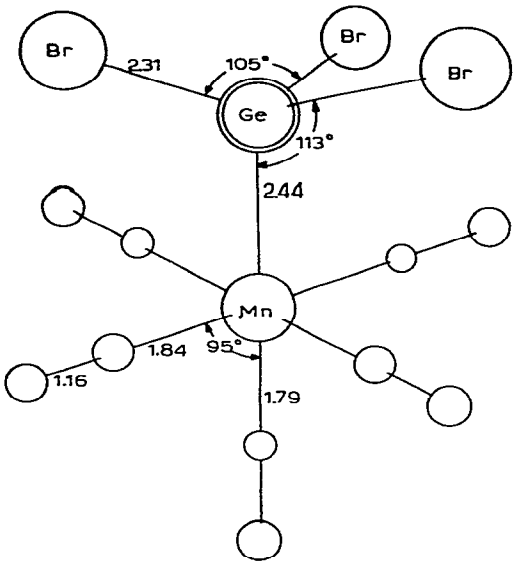

Fig. 1.

Br–Ge–Br 105° and Br–Ge–Mn 113°. The Mn atom co-ordination is distorted octahedral with the angles C_{axial}–Mn–$C_{equatorial}$ 95°.

It should be noted that the Ge–Mn bond length in the molecule $Br_3GeMn(CO)_5$ (2.44 Å) is considerably shorter than in $Ph_3GeMn(CO)_5$ (2.54 Å[11] and 2.60 Å[12]). The analogous shortening of a metal–metal bond with an increasing electronegativity of substituents bonded to a non-transition metal atom was found also in the series of other metal carbonyl derivatives containing bonds between a transition metal and an element of Group IVB[13].

The refinement of the structure is in progress.

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