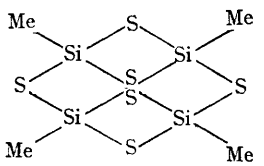
# The Structure of Tetra(methylsilicon) Hexasulphide

By J. C. J. BART and J. J. DALY*

(*Monsanto Research S.A., Eggbühlstrasse* 36, 8050 *Zürich, Switzerland*)

THE compound $(MeSi)_4S_6$ has been known for some time[1] and the first structure proposed[2] was the double four-membered ring form (I). This compound was later assigned[3] an adamantane structure (II) which was consistent with the spectroscopic data. The corresponding germanium compound $(MeGe)_4S_6$ has recently been synthesised[4] but in this case no decisive evidence was found in favour of either the adamantane or the four-membered ring structure.

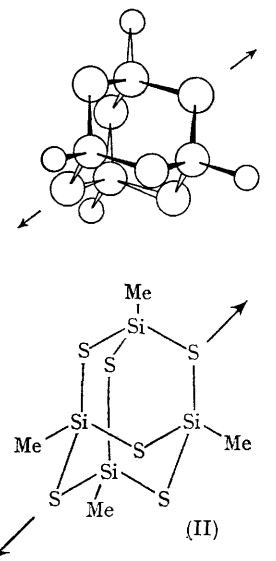



(I)

We have undertaken an *X*-ray analysis of $(MeSi)_4S_6$, which is iso-structural[4] with $(MeGe)_4S_6$, to establish the structure of these compounds. We later learned that another group had determined the structure of the germanium compound and the results of this analysis will be described[5] elsewhere.

Crystals of $(MeSi)_4S_6$ were supplied by Dr. K. Moedritzer of the Monsanto Company. They are monoclinic, space group $C2/c$, $a = 9{\cdot}382$, $b = 16{\cdot}513$, $c = 10{\cdot}584$ Å, $\beta = 107°10'$. The intensities of 1284 reflections measured on a linear diffractometer were used in the analysis. The structure was determined by direct methods and refined by least-squares with allowance for anisotropic temperature factors. The current *R* factor for 1284 planes is 0·054 and the hydrogen atoms have not yet been included in the calculations.

The analysis shows that the molecule has the adamantane structure (II) and possesses a two-fold symmetry axis. The molecules lie on the two-fold axes of the space group $C2/c$ ($Z = 4$). The Figure shows the molecule projected on to the *xy* plane and the Table gives average bond lengths and angles. The departures from the full tetrahedral symmetry $\bar{4}3m(T_d)$ are not large though they are statistically significant.




(II)

FIGURE. (*upper*). *The molecule projected on to the* xy *plane and* (*lower*) *the key to the drawing. The two-fold axis is shown.*

*Bond lengths* (Å) *and angles* (°)

| | e.s.d. in parentheses | | Range |
|---|---|---|---|
| Si—S | 2·128 | (0·002) | 0·012 |
| Si—C | 1·854 | (0·005) | 0·009 |
| ∠Si–Si–S | 104·5 | (0·1) | 0·1 |
| ∠S–Si–S | 111·8 | (0·1) | 1·6 |
| ∠S–Si–C | 107·0 | (0·2) | 1·3 |

(*Received, July* 11*th*, 1968; *Com.* 933.)

[1] Y. Etienne, *Bull. Soc. chim. France*, 1953, 791.
[2] Y. Etienne, *Angew. Chem.*, 1955, **67**, 753.
[3] J. P. Forstner and E. L. Mutterties, *Inorg. Chem.*, 1966, **5**, 552.
[4] K. Moedritzer, *Inorg. Chem.*, 1967, **6**, 1248.
[5] C. J. Fritchie jun., personal communication, 1968.