The extinctions indicate space group $Pnca$ and thus this compound is isostructural with $CaO.B_2O_3$ (Marezio, Plettinger & Zachariasen, 1963). Here the boron network consists of chains of triangularly coordinated boron groups.

$BaO.B_2O_3$ appears to have two polymorphic forms. At the moment, data are available only for the high-temperature form, which is rhombohedral. The cell dimensions referred to the hexagonal axis are $a = b = 7.23 \pm 0.01$, $c = 39.17 \pm 0.04$ Å. There is a marked halving of the c axis. The space group is either $R3c$ or $R\bar{3}c$.

The cell dimensions of all these crystals were obtained on a precession camera with Mo $K\alpha$ radiation $= 0.7107$ Å.

The data for the structure determination of $BaO.2B_2O_3$ were obtained with an integrating Weissenberg camera, with Mo $K\alpha$ radiation. The powder patterns were obtained with a diffractometer and Cu $K\alpha$ radiation.
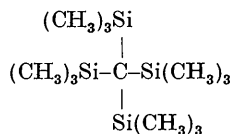
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Van der Waals radius and closest crystalline packing in the large spherical molecule, tetrakis(trimethylsilyl)methane. By R. L. MERKER and M. J. SCOTT, *Mellon Institute,* Pittsburgh 13, Pennsylvania, U.S.A.*

The synthesis of tetrakis(trimethylsilyl)methane recently accomplished in this laboratory will be the subject of a future publication. This large and spherically symmetrical molecule (the carbon analog of which has never been reported) possesses a surface comprised of twelve geometrically equivalent methyl groups:

$$(CH_3)_3Si$$
$$|$$
$$(CH_3)_3Si{-}C{-}Si(CH_3)_3$$
$$|$$
$$Si(CH_3)_3$$

It is a crystalline material which appears from visual observations to undergo a phase transition to another solid form at about 195–210 °C. Under atmospheric conditions sublimation occurs without true melting. Such behavior appears analogous to that of many spherically symmetrical molecules in which free rotation of the molecule within the crystal lattice can readily occur (Pauling, 1930; 1945, p. 375).

X-ray powder data have shown tetrakis(trimethylsilyl)-methane to be face-centered cubic with $a = 12.96 \pm 0.08$ Å. The calculated density for $Z = 4$ was found to be 0.929 g.cm^{-3} which is in good agreement with the observed value of 0.9113 g.cm^{-3}.

From the X-ray data, assuming that the molecules behave as rigid spheres without interpenetration, the molecular radius (r_1), which is the sum of the average distance from the center of the central carbon atom to the center of a hydrogen atom (r_2) and the van der Waals radius (r_3)† between this hydrogen and a peripheral hydrogen atom of a neighboring molecule, was calculated to be 4.58 Å.

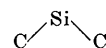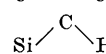From the bond angles and bond distances in tetra-methylsilane tabulated in Table 1, the average distance

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* Multiple Fellowship on Silicones Sustained by Dow Corning Corporation and Corning Glass Works.

† Actually r_3 represents one half the distance between spheres of radius r_2. To a first approximation this is one half the distance between hydrogen nuclei or van der Waals radius.

(r_2) from the center of the central carbon atom to the center of a peripheral hydrogen atom was determined to be 3.53 Å.

Table 1. *Bond distances and angles in* $(CH_3)_4Si$

Bond distances

Si–C	1.888 ± 0.02 Å ⎫	(Sheehan & Schomaker,
C–H	$1.10\ \pm 0.05$ Å ⎭	1952)

Bond angles

$\overset{Si}{\underset{C\diagup\ \diagdown C}{\diagup\ \diagdown}}$	109°	(Pauling, 1945, p. 85)
$\overset{C}{\underset{Si\diagup\ \diagdown H}{\diagup\ \diagdown}}$	$110 \pm 3°$	(Sheehan & Schomaker, 1952)

From this the van der Waals radius (r_3) was calculated to be 1.05 Å, the distance between hydrogen nuclei being 2.10 Å. This compares favorably with van der Waals radii determined for crystalline methane (1.002 Å) and ethane (1.165 Å) from X-ray analysis (Mack, 1932) and with the mean value of the intermolecular hydrogen radius (1.17 ± 0.02 Å) determined from later work with well defined structures containing the C–H bond (Kitaigorodskii, 1961).

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