

# High-pressure Synthesis of Strontium Hexasilicide

Aron Wosylus, Yurii Prots, Ulrich Burkhardt, Walter Schnelle, Ulrich Schwarz, and Yuri Grin

Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, D-01187 Dresden, Germany

Reprint requests to Dr. Ulrich Schwarz. E-mail: schwarz@cpfs.mpg.de

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The binary phase  $\text{SrSi}_6$  was prepared at a pressure of 10(1) GPa and a temperature of 1520(150) K. Single crystal refinements and powder diffraction data reveal that the compound crystallizes in the orthorhombic crystal system ( $Cmcm$ ,  $a = 4.4692(4)$ ,  $b = 10.256(1)$ ,  $c = 11.698(1)$  Å) and is isopointal to  $\text{EuGa}_2\text{Ge}_4$  and  $\text{EuSi}_6$ . Exothermic decomposition of the compound into  $\text{SrSi}_2$  and Si at 797 K and ambient pressure indicates that the compound is a metastable high-pressure phase. Analysis of the chemical bonding using the electron localization function and calculated charge densities reveals covalent bonding within the polyanion of four-bonded silicon atoms. Strontium cations are enclosed in the 3D net resulting in an electron balance  $\text{Sr}^{2+}[\text{Si}^0]_6^{2-}$ . In the electronic density of states the excess electrons of the framework are assigned to a filling of antibonding bands.  $\text{SrSi}_6$  is a metallic conductor with an electrical resistivity of  $\rho \approx 250 \mu\Omega\cdot\text{cm}$  at 300 K. Magnetization measurements indicate diamagnetic behaviour ( $\chi_0 = -50 \cdot 10^{-6} \text{ emu}\cdot\text{mol}^{-1}$ ).

*Key words:* Strontium, Silicon, High Pressure, Zintl Phase