

## **Rhombohedral (9R) and hexagonal (6H) perovskites in barium silicates under high pressure**

**HITOSHI YUSA,<sup>1,\*</sup> NAGAYOSHI SATA,<sup>2</sup> AND YASUO OHISHI<sup>3</sup>**

<sup>1</sup>Advanced Nano Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Ibaraki, Japan

<sup>2</sup>Institute for Frontier Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology, 2-15, Natsushima-cho, Yokosuka, 237-0061, Kanagawa, Japan

<sup>3</sup>Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo-cho, 679-5198, Hyogo, Japan

### **ABSTRACT**

Rhombohedral (9R) and hexagonal (6H) perovskites in BaSiO<sub>3</sub> were observed by using in-situ X-ray diffraction methods in high-pressure conditions. The 9R perovskite was found after successive laser heating at 27.9 GPa, and the 6H phase was identified at 48.5 GPa after laser annealing. No intermediate phase between the 9R and 6H phases was found in the pressure range between 27.9 and 48.5 GPa. These phases could not be recovered during decompression at room temperature and became amorphous at ambient pressure. The 9R and 6H structures are characterized by the periodicity of the stacking sequence of edge- and corner-sharing SiO<sub>6</sub> octahedra. In terms of the length of the O-O distance, the face-sharing SiO<sub>6</sub> octahedron in BaSiO<sub>3</sub> perovskite is the most distorted among oxide hexagonal perovskites.

**Keywords:** Perovskite, high pressure, barium silicate, Rietveld method