

## **Experimental evidence of sixfold oxygen coordination for phosphorus**

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### **ABSTRACT**

Phosphorus, a group V element, has always been found so far in minerals, biological systems, and synthetic compounds with an oxygen coordination number of four (i.e., PO<sub>4</sub> groups). We demonstrate using phosphorus *K*-edge XANES spectroscopy that this element can also adopt a sixfold oxygen coordination (i.e., PO<sub>6</sub> groups). This new coordination was achieved in phosphorus-doped (1 wt% P<sub>2</sub>O<sub>5</sub> level) SiO<sub>2</sub>-stishovite synthesized at 18 GPa and 1873 K and quenched to ambient conditions. This change of phosphorus coordination at high pressure within a dense silicate structure is particularly relevant to phosphorus mineralogy (and geochemistry) in the deep Earth. With a mantle abundance below 0.25 wt%, phosphorus has been shown to be mainly hosted by silicates (e.g., olivine) in the Earth's upper-mantle, in the fourfold-coordinated silicon sites. In the lower mantle where all silicon is sixfold coordinated, we show here that phosphorus has the crystal-chemical ability to remain incorporated into silicate structures.

**Keywords:** Phosphorus, coordination, XANES, stishovite, berlinite, lower mantle