

Experimental evidence of sixfold oxygen coordination for phosphorus

**FABRICE BRUNET,^{1,*} ANNE-MARIE FLANK,² JEAN-PAUL ITIÉ,² TETSUO IRIFUNE,³ AND
PIERRE LAGARDE²**

¹Laboratoire de Géologie, CNRS-ENS—UMR8538, 24 rue Lhomond, 75005 Paris, France

²Synchrotron-SOLEIL, BP48, 91192 Gif s/Yvette, France

³Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan

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., PO₄ groups). We demonstrate using phosphorus *K*-edge XANES spectroscopy that this element can also adopt a sixfold oxygen coordination (i.e., PO₆ groups). This new coordination was achieved in phosphorus-doped (1 wt% P₂O₅ level) SiO₂-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