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## Iron phosphate glasses: Bulk properties and atomic scale structure

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## Abstract

The bulk properties such as glass transition temperature, density and thermal expansion of iron phosphate glass compositions, with replacement of Cs by Ba, are investigated as a surrogate for the transmutation of <sup>137</sup>Cs to <sup>137</sup>Ba, relevant to the immobilisation of Cs in glass. These studies are required to establish the appropriate incorporation rate of <sup>137</sup>Cs in iron phosphate glass. Density and glass transition temperature increases with the addition of BaO indicating the shrinkage and reticulation of iron phosphate glass network. Average thermal expansion coefficient reduces from 19.8 x 10<sup>-6</sup> K<sup>-1</sup> to 13.4 x 10<sup>-6</sup> K<sup>-1</sup>, when 25 wt. % of Cs<sub>2</sub>O was replaced by 25 wt. % of BaO in caesium loaded iron phosphate glass. In addition to above bulk properties, the role of Ba as a network modifier in the structure of iron phosphate glass is examined using various spectroscopic techniques. The Fe<sup>II</sup> content and average coordination number of iron in the glass network was estimated using Mössbauer spectroscopy. Fe<sup>II</sup> content in the un-doped iron phosphate glass and barium doped iron phosphate glasses were 20, 21 and 22  $\pm 1$  % respectively and the average Fe coordination varied from  $5.3 \pm 0.2$  to  $5.7 \pm 0.2$  with increasing Ba content. The atomic scale structure was further probed by Fe K-edge X-ray absorption spectroscopy. The average coordination number provided by extended X-ray absorption fine structure spectroscopy and X-ray absorption near edge structure was in good agreement with that given by Mössbauer data.

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