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# Structure and properties of barium borophosphate glasses modified with molybdenum oxide

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## Abstract

Borophosphate glasses belong among important classes of glassy materials because they offer better thermal stability and chemical durability than phosphate glasses. Doping borophosphate glasses by heavy metal oxides like MoO<sub>3</sub> and WO<sub>3</sub> is interesting due to their semi-conducting properties ascribed to the presence of transition metal ions in multivalent states. In this study we prepared glassy samples from the BaO-P<sub>2</sub>O<sub>5</sub>-B<sub>2</sub>O<sub>3</sub>-MoO<sub>3</sub> system in two compositional series (100-x)[0.5PbO-0.4P<sub>2</sub>O<sub>5</sub>-0.1B<sub>2</sub>O<sub>3</sub>]-xMoO<sub>3</sub> and 80[0.5BaO-yB<sub>2</sub>O<sub>3</sub>-(0.5-y)P<sub>2</sub>O<sub>5</sub>]-20MoO<sub>3</sub>. Glasses were prepared from analytical grade BaCO<sub>3</sub>, MoO<sub>3</sub>, H<sub>3</sub>BO<sub>3</sub> and H<sub>3</sub>PO<sub>4</sub> using a total batch weight of 30g. The synthesis was carried out in platinum crucibles by heating up to 1000-1200°C. Physical properties of glasses were determined as well as their thermal behavior. For structural studies <sup>31</sup>P and <sup>11</sup>B MAS NMR spectroscopies were applied as well as Raman spectroscopy. <sup>31</sup>P MAS NMR spectra showed on the depolymerization of phosphate chains with increasing MoO<sub>3</sub> content due to the formation of Mo-O-P bonds between octahedral MoO<sub>6</sub> structural units and tetrahedral PO<sub>4</sub> units. <sup>11</sup>B MAS NMR spectroscopy is able to supply information on the boron coordination in the studied glasses because these spectra possess an ability to discriminate between tetrahedral BO<sub>4</sub> boron coordination and trigonal BO<sub>3</sub> coordination due to the different ranges of chemical shift values for BO<sub>4</sub> and BO<sub>3</sub> units. The measurement of <sup>11</sup>B MAS NMR spectra of the studied glasses with the NMR spectrometer with a high resolution (magnetic field 18.8T) revealed the formation of several different BO<sub>4</sub> structural units containing B-O-P, B-O-B and B-O-Mo bonds. The decomposition of these spectra brought relative amounts of individual mixed structural units in these glasses.

**Keywords:** phosphate glasses, glass structure, Raman spectra, NMR spectra

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