

## Poster Presentation

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### *Low temperature phase transition and structure of CsMgPO<sub>4</sub>*

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CsMgPO<sub>4</sub> doped in radioisotopes is a promising compound for usage as a radioactive medical source. However, a low temperature phase transition at the temperatures close to ambient conditions (-37°C) was observed. Information about structural changes is important in order to understand whether it can cause any problem for medical use of this compound. Structural changes have been investigated in detail using synchrotron powder diffraction methods, Raman spectroscopy and DFT calculations. The structure undergoes transformation from orthorhombic modification, sp. gr. Pnma (RT phase) to monoclinic modification, sp.gr P21/n (LT phase). New LT modification adopts similar to RT but slightly distorted unit cell: a=9.58199(2)Å, b=8.95501(1) Å, c=5.50344(2)Å, β=90.68583(1)°, V=472.198(3) Å<sup>3</sup>. The framework is made up of alternating magnesia and phosphate tetrahedra sharing vertices with caesium counter cations located in the channels formed. Upon the transformation a combined rotation of PO<sub>4</sub> and MgO<sub>4</sub> tetrahedral takes place. A comparison with other phase transition in ABW-type framework class compounds is given.

**Keywords:** phase transition, ab-initio structure solution, synchrotron powder diffraction