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### Compressibility and electronic structure variation with pressure for $\text{EuVO}_4$ : A combined experimental and computational study

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Europium orthovanadate,  $\text{EuVO}_4$ , crystallizes in the zircon-type structure (space group  $I4_1/amd$ ,  $Z = 4$ ) under ambient conditions and is known to transform to a scheelite-type structure at about 8 GPa. The equation of state of this compound has already been studied. However, the reported experimental and theoretical values of the bulk modulus exhibit a considerable scatter, for both, the zircon and scheelite-type polymorphs. As for the dependence of the electronic structure with pressure, such data have not been reported yet.

In the present study, structural, elastic and electronic properties of zircon-type and scheelite-type europium orthovanadate are investigated experimentally, by *in-situ* X-ray diffraction using synchrotron radiation, and theoretically within the framework of the density functional theory (DFT). The obtained results on bulk modulus show a perfect agreement of experiment with theory. Discrepancies between the present values and those earlier reported ones are attributed to differences in the details of the experimental procedure. The calculated band structure confirms that zircon-type europium orthovanadate is a direct-gap semiconductor, with a band-gap energy at zero pressure of 2.88 eV. The variation of electronic structure and of the bandgap with pressure is determined.

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### Energy transfer processes to $\text{Eu}^{3+}$ ions in $\text{K}_5\text{Li}_2\text{GdF}_{10}$ doped with $\text{Eu}^{3+}$ , $\text{Pr}^{3+}$ , $\text{Tb}^{3+}$ and $\text{Dy}^{3+}$ upon VUV excitation

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The X-ray examination of small crystals of  $\text{K}_5\text{Li}_2\text{LnF}_{10}$  ( $\text{Ln} = \text{La}-\text{Gd}$ ) has proved that the materials crystallize in a form of single phase. It is orthorhombic (space group  $D_{2h}^{16}-Pnma$ ), the unit-cell parameters are  $a = 20.775 \text{ \AA}$ ;  $b = 7.882 \text{ \AA}$ ;  $c = 6.963 \text{ \AA}$ ; for  $\text{Ln} = \text{La}$ .

The crystal structure is built from layers perpendicular to the  $a$  axis, formed by  $\text{LnF}_8$  dodecahedra and  $\text{LiF}_4$  tetrahedra. Rare-earth ions and lithium ions occupy sites with  $C_5$  symmetry, whereas potassium and fluorine ions occupy sites with  $C_5$  and  $C_1$  symmetry. The crystal structure is uncommon in that the  $\text{LnF}_8$  polyhedra do not share fluorine ions and the nearest rare-earth ions are separated by more than 6.8  $\text{ \AA}$ . Owing to these features, exchange interactions between rare-earth ions may be neglected and multipole interactions are expected to be strongly reduced. Such a conditions allows to analyze rather pure multipole interactions between ions.  $\text{Pr}^{3+}$ ,  $\text{Tb}^{3+}$  and  $\text{Dy}^{3+}$  possesses metastable multiplets situated in the blue area of the spectrum that should transfer the energy to the low positioned  $\text{Eu}^{3+} \text{ } ^5\text{D}_0$  one [1].

The  $\text{Pr}^{3+}$  ion can work as a sensitizer of  $\text{Eu}^{3+}$  luminescence from the  $^5\text{D}_0$ . It has been discovered that the  $\text{Pr}^{3+}$  ions to transfer an energy to the  $\text{Eu}^{3+}$  ions needs the presence of  $\text{Gd}^{3+}$  ions. In  $\text{K}_5\text{Li}_2\text{LaF}_{10}$  system only a luminescence of  $\text{Pr}^{3+}$  was observed upon excitation of f-d bands of praseodymium [2]. It can suggest that excited the  $\text{Pr}^{3+}$  ions very efficiently transfer the energy to  $\text{Gd}^{3+}$  ions. Such an efficient energy transfer has been observed in other system  $\text{YF}_3:\text{Pr}^{3+}$ ,  $\text{Gd}^{3+}$  [18]. At low temperature emission spectra (not shown here) the  $\text{Pr}^{3+}$  f-f emission upon UV-VUV excitation was observed. It suggests that energy transfer from d levels of  $\text{Pr}^{3+}$  to  $\text{Gd}^{3+}$  states is thermally dependent.

In the case of  $\text{Dy}^{3+}$  ions, no transfer upon excitation into f-d bands of  $\text{Dy}^{3+}$  was observed to  $\text{Gd}^{3+}$  or  $\text{Eu}^{3+}$  ions. Dysprosium is rather independent. As well as no transfer from  $\text{Dy}^{3+}$  to other ions was not observed, no efficient transfer to the  $^4\text{F}_{9/2}$  multiplet of  $\text{Dy}^{3+}$  was observed.

The best results was found for  $\text{Tb}^{3+}+\text{Eu}^{3+}$  system. It occurs that upon excitation into f-d transitions bands of  $\text{Tb}^{3+}$  an efficient luminescence from  $\text{Eu}^{3+}$  can be observed in  $\text{K}_5\text{Li}_2\text{GdF}_{10}$  an  $\text{K}_5\text{Li}_2\text{LaF}_{10}$  matrixes. What is more upon excitation of  $\text{Tb}^{3+}$  ions below the d levels no efficient energy transfer from  $\text{Tb}$  to  $\text{Eu}$  was observed. Such an observation is validated with analysis of the decay curves of  $\text{Tb}^{3+}$  luminescence.