

## Structural and Luminescence Peculiarities for Scheelite-Related Binary Molybdates

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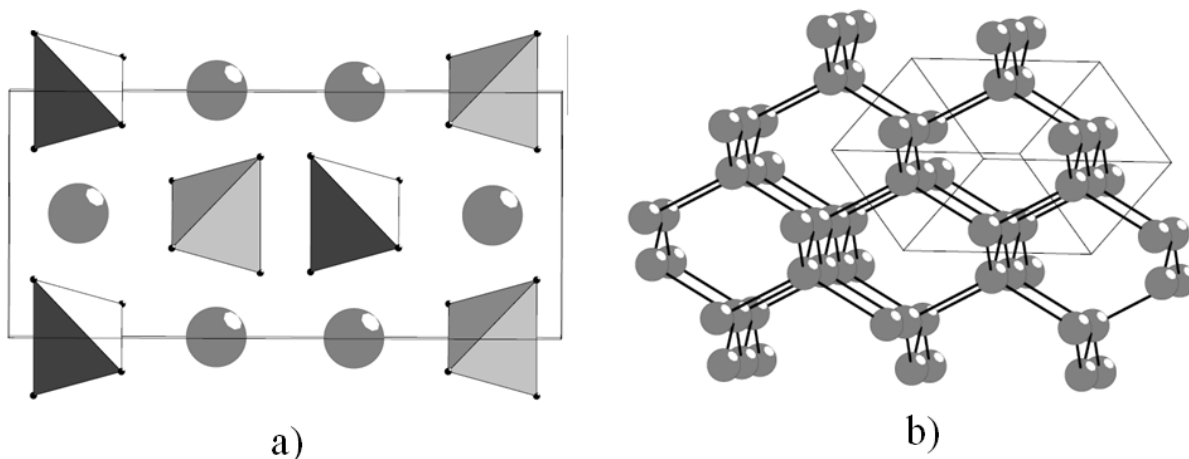
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Pure and doped scheelite-related oxides containing rare-earth metals and molybdate or tungstate anions have been intensively studied during the past decade due to their attractive structures and topologies as well as their potential applications in luminescence and optics [1-2]. Although numerous complex derivatives from the ideal tetragonal structure *e* (space group  $I4_1/a$ ,  $Z = 4$ ) have been synthesized, rational theory about the relationship between the structures and the components constructing them has not been developed yet.

Having general chemical formula  $(M_{0.5}RE_{0.5})MoO_4$ , where *M* – is alkaline metal and *RE* – rare-earth one, both metals are located in  $(M,RE)O_8$  dodecahedra, which constitute square antiprisms, while molybdenum ions have a tetrahedral oxygen environment  $MoO_4^{2-}$  with almost equal cation–oxygen interatomic distances (Fig. 1a). Due to the statistical distribution of alkaline and rare-earth metals within the crystallographic sites of the scheelite structure these crystals provide large bandwidths of the optical absorption and luminescence bands of rare-earth ions. Alternatively the crystal structure can be regarded as a regular intergrowth of these metals in a way of diamond-like framework (fig.1b).

On the basis of structure determination from single crystal data and luminescence properties of a number of binary molybdates the peculiarities of crystal structure – luminescence relationships are explored for isostructural compounds  $KCeMo_2O_8$  and  $KPrMo_2O_8$ . The key trends in scheelite –related structural motifs are compared for known luminescent hosts with common building blocks.



**Fig.1.** a) The typical representation of the scheelite unit cell and b) formation of diamond-like architecture by rare-earth metals network

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 [2] G.M. Kuz'micheva, I.A. Kaurova, V.B. Rybakov, P.A. Eistrikh-Geller, E.V. Zharikov, D.A. Lis, K.A. Subbotin, *Cryst. Eng. Comm.* **18** (2016) 2921-2928.