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Assessment on the PhD thesis submitted by Anna
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The submitted thesis with the title Crystal chemistry of natural and synthetic titanium and molybdenum oxocompounds represents a doctoral dissertation in cumulative form, thematically compiled of five scientific articles published in internationally recognized journals. The main focus of the overall objective is the crystal chemistry and structural crystallography on representatives of this class of compounds, which are of particular interest for nuclear waste management. Molybdate solids are supposed to play a role in oxidation processes of high-level nuclear waste, while titanates are considered for immobilization of radionuclides.

Within the scope of this PhD thesis the objective of the experimental study are investigations of selected compounds, such as cesium molybdates and titanites of the pyrochlore-murataite series. Experimental investigations encompass the synthesis of individual compounds by hydrothermal reactions or high-temperature reactions, chemical analyses by means scanning electron microscopy, extensive investigations by means of single-crystal X-ray diffraction methods, and electron microscopy. Later methods were applied in order to characterize details of the atomic structure and to record and resolve crystallographic features such as of superstructure reflections and diffuse scattering involved. The results of these experimental investigations comprise knowledge on the crystalchemistry of new alkali-(poly)molybdates, i.e. β - $\text{Cs}_2\text{Mo}_4\text{O}_{13}$, $\text{Cs}_3(\text{Mo}_2\text{O}_7)$, organometallic octamolybdates of the type $[\text{emin}]_3\text{M}^+(\text{Mo}_8\text{O}_{26})$. Moreover synthetic murataites following different polytypic variations (-3C, -8C) have been investigated and structural models of complex superstructures of this modular structure family have been presented.

All five scientific articles are published in internationally recognized journals, such as: Acta Crystallographica (Section E), Inorganic Chemistry Communications, Radiokhimiya (in Russian), and Zeitschrift für Kristallographie, which are ranging with impact factors between 0.347 (Acta Cryst E) and 2.016 (Inorg Chem Comm). All articles are published between 2009 and 2013, with four of the five articles referenced with the candidate as first author. The contributions of the candidate is stated for each publication and comprise the synthesis, measurement and data analyses to be carried out in own responsibility or in a leading role, and in most cases also the writing with considerable support of the co-authors. As the process of submission to scientific journals the contributions involves critical review, the acceptance to publication implies that an appropriate check of the quality of the presented science has been sufficiently carried out. Surveying under the same aspect the accepted articles, there is no additional comment necessary to be made, and each of the articles represents a piece of solid scientific work based on careful experimental studies.

This assessment also applied to the lead paragraphs describing background, motivation, and objectives and which give an concise overview on the individual results. These lead paragraphs are written in a form, which is easy to understand, which outline the main points and which gives appropriate references to the previous work in this field.

In summary it can be said, that the submitted thesis represents high-rank research, from scientific point of view both the articles and the thesis itself undoubtedly confirm the qualification of the candidate of having fulfilled the requirements for obtaining a PhD degree, which compares to international standards. Therefore I finally want to express my unrestricted recommendation to the responsible advisory board to continue and complete the ongoing process.

Ronald Miletich-Pawliczek