Evaluation of the thesis by Anna S. Pakhomova
"Crystal chemistry of natural and synthetic titanium and molybdenum oxocompounds"

The basic requirement for the geological formation as a repository for the disposal of radioactive waste is its capability to contain and isolate the radionuclides from the biosphere. One of the most promising technologies is the production of synthetic minerals which incorporate high-level waste within low solubility crystalline lattices. As per this concept, titanates and titanosilicates of different structure types are considered to be very interesting compounds because they can accommodate a wide range of cation substitutions, possess very good selective properties, and are characterized by a high radiation resistance. The thesis of Anna Pakhomova is dedicated to the research of titanate minerals and their synthetic analogues using X-ray structural analysis in order to give crystal chemical interpretation of studied phases as matrices of possible materials for the disposal of HLW in geological repositories. Natural and synthetic molybdates studied by the author represent an alternative, but not less important, group of compounds: several molybdates have been found in spent nuclear fuel.

An essential material of this work is crystal structures of the mineral laachite, five molybdates synthesized by the author, and two synthetic modifications of mineral murataite. All eight structural studies were done on the basis of mono crystal X-ray diffraction. The methods of investigation used are up-to-date and, as far as I can judge, the results are scientifically sound. Provided crystal chemical analysis looks reasonable and permits comparing new data with previously found for related compounds. Very interesting conclusions have been made for a series of "murataites" interpreted by the author in terms of modular concept. The structural transformation from pyrochlore to murataite achieved through intermediate polysomes has been well elaborated by the author.

However, there are some points which in my opinion deserve additional comments or corrections. The most important objection is connected with a representation of data received for the mineral laachite. A half page of text that should provide details regarding this mineral crystal structure and peculiarities of its crystal chemistry (no mineral formula given!) is obviously not enough for full understanding and adequate evaluating of presented results. The promised original paper appended to the end of the thesis (page 13) is actually absent. The reviewer could not find complete information in the literature: one page of abstract (Volume of abstracts. The 2nd International Conference "Clays, Clay Minerals and Layered Materials". Russia, Saint-Petersburg, 2013, p.42) cannot give necessary fine points.

Additional doubts arise after considering the data presented in the section with murataite-3c description. I cannot accept standard deviations equal to 57, 47, 154 and similar in coordinates, interatomic distances, or volume; in my opinion these values have little sense, as well as a value of extinction coefficient equal to 0.00001(3).

Some minor points that might be simple typos are as follows. 1. The same amount (2218) of total measured and unique reflections shown in Table 1 (page 14) in connection with the $Cs_2Mo_4O_{13}$ crystal structure could hardly be realistic. 2. The lack of "PIV" paper and presence of two identical pages with its reference and the authors' contribution details instead. 3. "Imaging", not "Image" (pages 15, 21) plate area detector.

The above comments are not written in the spirit of disparagement and do not call into question the overall satisfactory character of the dissertation under review. The author Anna S. Pakhomova deserves praise for her achievements and should be awarded the Ph.D. degree.

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