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Report of the member of the dissertation board for the dissertation of
Taras Leonidovich Panikorovskii
on the topic:
"THE CRYSTAL CHEMISTRY OF VESUVIANITE GROUP MINERALS"
submitted for a Ph.D. degree in science 25.00.05.

As the title of the PhD Thesis promises, the investigations of Taras Leonidovich Panikorovskii cover a multimethodological approach applying mineralogical, chemical, physical and crystallographic techniques to differentiate the diversity of vesuvianite group minerals.

Vesuvianites comprise a complex and wide spread group of rock forming silicate minerals. In the past, the structural and related chemical complexity of this mineral group has hampered a comprehensive treatment of the subject. In particular, general rules were missing allowing detailed classification. This gap is excellently filled by the presented dissertation. In order to shed light at the diverse existing picture of the chemical and structural variations, the author studied the huge amount of 170 samples of vesuvianite-group minerals from various world-wide deposits. The analytical techniques used were (1) single crystal X-ray diffraction studies (2) powder X-ray diffraction analysis (3) infrared spectroscopy (4) differential scanning calorimetry (5) investigation of optical properties (6) determination of chemical composition and electron microprobe measurements (7) ICPMS = Inductively Coupled Plasma - Mass Spectrometry (8) photoelectron spectroscopy (9) Mössbauer spectroscopy and (10) solid-state NMR investigations. It is obvious that such a variety of techniques was not available in the home institution of the PhD candidate but required intensive collaboration with additional laboratories and specialist scientists. Such collaborations are highly appreciated because they do not only expand the horizon of a scientist but also support team-working abilities, most important for complex issues and a multimethodological approach.

The basis of the submitted thesis are 9 papers by Panikorovskii as first author published between 2016 and 2017 in Russian and international peer reviewed journals, complemented by additional 5 abstracts or recent full papers either published or accepted with Panikorovskii as one of the co-authors. Even if not subject of the written thesis but nevertheless important for evaluation of the scientific impact and merit of his investigation is the fact that Panikorovskii was unanimously confirmed as chairman of a working group elaborating a report on the nomenclature for the vesuvianite-group minerals to be proposed to the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association. This report, which is close to completion, distinguishes three subgroups comprising 11 vesuvianite group minerals of which 6 were discovered in the course of this evaluated thesis. Furthermore, the discovered relations between crystal

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structure, chemical composition and properties of vesuvianite group minerals, compiled in the thesis of Panikorovskii, are key issues of the upcoming nomenclature report.

The detailed thesis of 197 pages Russian text with an additional appendix of ca. 90 pages containing tables, is very well organized and written. Furthermore, the Russian text and appendix are translated into English, thus the complete thesis comprises 566 pages. The English translation, which is highly appreciated, is rather rough and bumpy in style, grammar, and orthography but fulfills its goal. Unfortunately, it contains few wrong translations in comparison with the original Russian text: e.g., the Russian term for "isolated tetrahedra" is mistranslated into "sorosilicate" and the Russian term "diorthogroup" is mistranslated into "nesosilicate". However, this translational confusion is for the reader very obvious because the labels of the tetrahedral sites are also given.

The thesis consists of four thematically coordinated main chapters bracketed by an introduction and a conclusion chapter. The introduction not only contains a condensed historical overview on the today's knowledge about vesuvianite group minerals but also defines goals, objects, novelty, significance, and eight thesis statements to be defended. The latter statements are concise rules derived from the mineral complexity and corresponding crystal chemical correlations worked out in the course of the thesis.

The first chapter of the thesis "1. *Mineralogical, petrological and structural diversity of vesuvianite-group of minerals*" is intended to summarize the "status quo" of knowledge on vesuvianite minerals after completion of the thesis. There are various sub-chapters, starting with "*Petrological Diversity*". Except the general division into vesuvianite occurrences in regional metamorphic and contact metamorphic rocks, the thread of this subchapter is a little bit difficult to follow and not always on the point. In the foreground of the corresponding text is most notably a description of the chemical diversity of vesuvianite in various rock types but not so much a profound analysis of different underlying petrological conditions. This slight weakness is more than balanced by the excellent subchapters "*Chemical Variations*" and the associated chapters on the crystal chemistry. Here the author demonstrates his main competence and interest displaying convincing trends with histograms of elemental frequencies and correlation diagrams presenting the basis of the observed homeo- and hetero-valent substitutions, hydrogen bonding, polyhedral distortions, structural varieties etc. All these issues are nicely explained and supported by detailed structural drawings. Clear guidelines are presented how structural varieties may be distinguished from a single-crystal diffraction pattern showing evidence of different space-group symmetries, identified by symmetry violations of specific groups of observed reflections.

The second Chapter "2. *Experimental methods*" summarizes details about the 10 experimental methods applied and provides the source of the sample origin of the 170 studied specimens. Ca. 70% came from museum collections and 30% from private collectors.

In the third chapter "3. Minerals of vesuvianite group" the analyzed vesuvianite group species are listed and discussed based on their specific properties as evaluated by the applied experimental techniques. This chapter is excellently prepared presenting detailed information about the interpretation of the experimental results. Specific properties are explained by easy to follow structural drawings. Following mineral species were analyzed: (1) vesuvianite, (2) wiluite and boron-bearing vesuvianite, (3) cyprin and Cu-bearing vesuvianite, (4) alumovesuvianite, (5) magnesiovesuvianite, (6) fluorvesuvianite and F-bearing vesuvianite, (7) manganvesuvianite, (8) hongheite, (9) Manaevite-(Ce) and *REE*-bearing vesuvianite, and

(10) milanriederite. In summary, this chapter is the main basis of the upcoming nomenclature report, addressed above, finalized under the chairmanship of T.L. Panikorovskii.

Chapter 4. "Mechanisms of cooperative crystal-chemical adaptation in the vesuvianite structure as the basis of its homeostasis" is for me the absolute highlight of the dissertation. Here the general experience from the detailed analyses of 170 specimens is summarized to substitution rules and their influence on structural modifications and distortions. In addition, specific examples are discussed in detail, which facilitates comprehension. Initially I was puzzled by the term homeostasis (also used in the Russian original version), which I have not yet encountered in connection with mineralogy in English written literature. A short explanation may have been useful in the text (e.g. homeostasis denotes an equilibrium condition of an open dynamic system, maintained by an internal regulating process). After understanding the meaning of the term, originally used in biology and physiology, I have to confess that it perfectly describes the summarized findings in chapter 4.

The final conclusions of the thesis are summarized in form of 10 concise statements also presenting an outlook what we have to expect concerning complexity and new species in the field of crystal chemistry of vesuvianite group minerals.

In summary, I evaluate the thesis of Taras Leonidovich Panikorovskii entitled "THE CRYSTAL CHEMISTRY OF VESUVIANITE GROUP MINERALS" as **outstanding on an international level** in terms of quality, detailedness, effort, diligence, and impact on general crystal chemistry of minerals. For this reason, I have no doubt that it complies with the meets of the basic requirements set by the Order of 01.09.2016 No. 6821/1 (On the order of awarding degrees at St. Petersburg State University).
Taras Leonidovich Panikorovskii deserves to be awarded Ph.D. in Science 25.00.05.

Member of the Dissertation Board

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