

REVIEW

in competition for the academic position of “Professor”
in the professional field 4.4 “Earth Sciences” (Mineralogy and Crystallography)
for the needs of the department “Structural Crystallography and Materials Science”
at the Institute of Mineralogy and Crystallography “Acad. Iv. Kostov” (IMC) - BAS,
Announced in the State Gazette, no. 95/14.11.2023 г.

Reviewer. *Prof. Prof. Vilma Petkova Stoyanova, IMC-BAS, member
of the scientific jury under Order No. 28 RD-09/10.01.2024.*

Candidate: Prof. Dr. Rositsa Hristova Titorenkova, IMC-BAS

1. Information about the competition

The competition for the academic position (AD) “Professor” in the professional field 4.4. “Earth Sciences” (Mineralogy and Crystallography) is announced for the needs of the department “Structural Crystallography and Materials Science” at the Institute of Mineralogy and Crystallography “Acad. Iv. Kostov” (IMC) - BAS in the "State Gazette" issue 95/14.11.2023. Within the deadline regulated by the Law on the Development of Academic Staff in the Republic of Bulgaria and the Regulations of the IMC-BAS (in force since 21.10.2021), as the only candidate, submitted documents Assoc. Prof. Dr. Rositsa Hristova Titorenkova, who is on a basic contract in the same field at the IMC-BAS.

The procedure for the announcement of the competition is based on Article 19 (1) of the PPPRAS of the IMC-BAS and in accordance with the Order No. 28RD-09/10.01.2024 of the Director of the IMC-BAS for determining the composition of the NW. Following the first meeting of the JW on 24.01.2024, in accordance with Order No. 42RD-09/22.01.2024 of the Director of the IMC-BAS, I have been appointed to prepare a review of this competition.

1. Career development and professional qualities of the candidate

1.1. Brief biographical data

Assoc. Prof. Dr. Rositsa Hristova Titorenkova graduated in 1988 at Sofia University "St. Kliment Ohridski", Faculty of Geology and Geography (SU), Sofia. Sofia (Diploma, №111441/08.05.1990) as a Master of Science in Geology with professional qualification “Geologist-Chemist”. In 2007 he received the educational and scientific degree (PhD) “Doctor” in the scientific specialty “Mineralogy and Crystallography” (Diploma № 31191/01.03.2007, approved by Protocol No 6-04/15.12.2006 of the SAC) after successful defense of his dissertation.

The professional activity of Assoc. Prof. Prof. Titorenkova started in 1996 at the Institute of Applied Mineralogy - BAS as “Mineralogist – Specialist”. In 2013, after a successful competition, she was appointed to the position of “Associate Professor” at the Institute of Mineralogy and Crystallography “Acad. I. Kostov” - BAS. Since 2013 until now she is also the Head of the Laboratory “Spectroscopy” at IPM-BAS and also Scientific Secretary at the same Institute since 2013 until now.

1.2. Specialisations and courses

For the professional development of Assoc. P. Titorenkova's professional development has been substantially supported by numerous specializations and additional training courses in the

field of Earth Sciences and the mastery and application of spectroscopic methods, mainly Infrared and Raman spectroscopy, namely:

- 1996-1997 - at GI-BAS - Specialization “Statistical Methods in Geology”, scientific supervisor. Prof. Vasil Vachev (Mathematical Geology);
August - September 2004 - University of Vienna, Austria, European Mineralogical Union Summer School 6th EMU School “Spectroscopic Methods in Mineralogy”;
- September, 2006 - University of Karlsruhe, Germany, ATR infrared spectroscopy with synchrotron radiation;
- March, 2007 - University of Vienna, Workshop: ‘Vibrational Spectroscopy (Infrared Absorption and Raman): Applications in Geosciences’;
- June, 2009 - University of Bilbao, Spain, Crystallography online: International School on the use and application of the Bilbao Crystallographic Server;
- 28. 11. 2010 - 28. 11. 2012 - Yamaguchi University, Japan, Postdoctoral specialization with JSPS (Japan society for promotion of Science) scholarship;
- September, 2015 - December, 2015 - University of Hamburg, DAAD scholarship (German academic exchange service)

1.3. Membership in scientific organisations

Assoc. P. Titorenkova is a member of scientific organizations thematically related to her scientific profile, namely - Bulgarian Geological Society (http://www.bgd.bg/frames_home_BG.html) and Canadian Mineralogist of the Mineralogical Association of Canada.

1.4. Compliance of the submitted documents with the requirements for the academic position "Professor"

The candidate has submitted the application package for the AD Professor competition within the prescribed time limits.

1. **Set of documents (Article 19 (3) of the PPRAS of the IMC-BAS).** R. Titorenkova has submitted all the required documents for the academic position of "professor" in accordance with Art. 24, par. 1, items 1-5 of the Law on the Development of Academic Staff in the Republic of Bulgaria (Law on the Development of Academic Staff in the Republic of Bulgaria) (in force from 23.12.2022) and Art. 1 (1-5) of the Regulations for its Implementation (RAPRAS) (in force from 19.02.2019), as well as Article 18 (4) of the RAPRAS of the IMC-BAS (in force from 21.10.2021) within the established deadlines according to Report No. 36RD16/16.01.2024 of the Commission for the examination of the documents of the candidate for participation in the competition and the compliance of the documents in the competition for the AD “Professor”. The documents were also examined by the scientific jury at the first meeting on 24.01.2024, which decided to admit the candidate Assoc. Prof. Dr. Rositsa Titorenkova to the evaluation for the academic position “Professor” at IMC-BAS.
2. **Acquisition of the degree of Doctor of Education and Science (Art. 60 item 1 of the PPHRAS).** R. Titorenkova is registered in the NACID (<https://ras.nacid.bg/dissertation-preview/28104>), with a recognized educational and scientific degree "Doctor" on the basis of Diploma No/date: 31191/01.03.2007, approved by Protocol No/date: 6-04 / 15.12.2006, issued by the SAC, city of. No.. “Mineralogical features of zircon from Paleozoic metagranitoids in the Ograjden Mountains, Serbian-Macedonian Massif, SW Bulgaria”.
3. **Seniority of the academic position "Associate Professor" (Article 60(2) of the PPHRAS).** Titorenkova has held the academic position of Associate Professor for 10 years and 7 months in the professional field 4.4. Earth Sciences, which satisfies the requirement for more than 5

years of experience in the academic position of Associate Professor according to the requirements of Article 29, para. (in force from 23.12.2022).

4. **Published monographic work or equivalent publications in specialized scientific journals (Art. 60 item 3 of the PPHRAS).** The publications submitted for the competition are not duplicative of the publications for the PhD degree and for the post of Associate Professor and comply with the criteria for indicator groups "C" and "D" of the minimum national requirements of Article 1a(2) of the PPHRAS, Article 2(4.5) of the PPHRAS of the BAS and Article 2(3)(3) of the PPHRAS of the IMC-BAS.
5. **Reference for the fulfilment of the minimum national requirements (Article 60, paragraph 5 of the PPHRAS).** The applicant has attached a reference on the fulfilment of the minimum national requirements under Art. 2b, para. 1 and 3 of the RRBA , as well as the enhanced criteria under Article 11(6) of the RRBA and under Article 19(1) of the RRBA. 3(17) of the PPHRAS (in force from 21.10.2021) of the Institute of Mineralogy and Crystallography "Acad. Iv. Kostov, BAS.
6. **Information on plagiarism (Article 60, Section 6 of the PPHRAS).** P. Titorenkova for participation in this competition.

2. Evaluation of the scientific production and scientific metrics of Assoc. P. Titorenkova

2.1. Characteristics and evaluation of scientific publishing activities

Assoc. P. Titorenkova has provided a cumulative list of 82 scientific publications, 40 of them (48.8%) are in refereed and indexed international journals with impact factor (IF- Journal Citation Indicator - Q-JCI) and impact rank (SCR - SCImago Journal Ranking).

The number of publications of Assoc. P. Titorenkova for participation in the current competition is 36 according to the provided list of publications. I accept all the publications and will take them into consideration when preparing the review. The detailed scientific metric shows that 17 (47%) of the articles have been published in international journals, another 17 (47%) of them - in national journals, 2 of the publications are book chapters. According to the list of publications, Assoc. Titorenkova is a co-author of 27 (75%) scientific papers visible in the WoS and Scopus world databases of scientific information, of which 19 (53%) articles are in journals with impact factor, 5 (14%) - in journals with impact rank and 7 (19%) - in full text in conference proceedings and in journals without impact factor. The distribution of articles by quartiles of WoS and Scopus journals in which the publications are in is as follows: 10 (28%) articles are in Q1 journals; 5 (14%) - in Q2 journals; 2 (6%) - in Q3 journals and 5 (14%) - in Q4 journals, i.e. more than 60% of the scientific publications have undergone peer review and approval in indexed and refereed international journals. This is an excellent attestation of the quality and level of research involving Assoc. Titorenkova. High-ranked journals include *Journal of Raman Spectroscopy (Q1)*, *Ceramics International (Q1)*, *Journal of biomedical materials research Part A (Q1)*, *Gels (Q1)*, *Materials (Q2)*, *Microporous and Mesoporous Materials (Q1)*.

The data from the lists of publications demonstrate the scientific growth of Assoc. Titorenkova especially in recent years and reorientation of her publishing activity towards high-ranking publications, mainly with Q1, in areas corresponding to the objectives of this competition.

In the present competition the publications with which Assoc. In 5 of them she is the first author (in group "B" - № 2, 10; in group "G" - № 12, 17 and 28), in 9 she is the second author (in group "B" - № 1, in group "G" - № 11, 13, 14, 16, 27, 30, 31, 33), and in the rest (22 pieces) she is the third and next co-author. All papers were published in the last 10-12 years after 2011, and the largest number were in 2022 (12 ps.), 2019 and 2023 (7 ps.).

2.2 Characteristics of citations on publications

The total number of citations noted on the publications of Assoc. Titorenkova, presented in a separate list, is 442 according to the System for Reporting Scientific and Expert Activity at BAS - Sonix. Of these, 100 items, referenced and indexed in world-renowned databases of scientific information Scopus and WoS, were submitted for the requirements in the competition for AD "Professor" according to the citation reference. This citation is an objective indicator of the quality of the scientific production of Assoc. Titorenkova and proves the serious international response and interest in the results obtained in her works. The Hirsch index (h) according to Scopus is 9, for the publications of the competition, it is 6. The total number of points from citations in scientific journals refereed and indexed in world-known databases of scientific information Scopus and WoS, presented in the Reference for fulfillment of minimum criteria, is 500. This result exceeds more than 4 times the required 120 points even according to the increased requirements under the BAS and IMC-BAS PPPASRB.

2.3. Characteristics of participation in scientific forums

The scientific results of the research of Assoc. Titorenkova, obtained after obtaining the academic position of Associate Professor, have been promoted through 40 participations in 31 scientific forums (since 2012), of which 20 in international scientific forums and 11 in national forums. In the programme of these scientific forums the participation of Assoc. Titorenkova with 15 oral contributions - reports and lectures, and 25 poster contributions.

2.4. Characteristics of participation in research projects

Assoc. P. Titorenkova has an impressive participation in the project activities of IMC-BAS. She has actively participated in 23 national and international scientific projects, being a participant in 18 projects and a leader of 5. Of all the projects, 4 are international in bilateral cooperation between the academies of BAS and other related academies in the Czech Republic and Romania, and one is with Germany (DAAD German Academic Exchange Service), of which she is also the leader. The applicant does not provide evidence of project participation in the package, but only a list of project names and roles. There is also no reference to the funds involved in the projects.

2.5 Expertise and teaching

Together with the scientific research activity Assoc. Titorenkova is also active as a lecturer in a course on "Infrared Spectroscopy" and "Accessory Minerals-Indicators" at the Central Research Institute of BAS. She has taught students from the University of St. Kl. Ohridski in the course "Vibrational spectroscopy in mineralogy" in 2014-2016.

Assoc. Titorenkova is a scientific supervisor of 1 PhD student at IMC - D. "Structural characteristics of dental enamel studied by vibrational (micro-infrared and Raman) spectroscopy", who was discharged with the right to defend.

Assoc. Titorenkova is the supervisor of student G. Markov from Sofia University "St. Kliment Ohridski" during the period 2016-2017 under the "Student Practices" program.

Assoc. Titorenkova is also a lecturer in the course on Raman spectroscopy - International summer school, Centre of Applied Spectroscopy, Instrumental analysis, 15-21.07. 2013, Sofia

2.6. Assessment of the fulfilment of the minimum national requirements for the scientific field

4.4. Earth Sciences according to the BAS and IMC-BAS From the made reference it is established that the scientific production of Dr. Titorenkova is on the subject of the competition. The analysis of the submitted materials shows that it meets, and in some indicators exceeds, the national

requirements (ZRACPB*), as well as the increased criteria of the Bulgarian Academy of Sciences and the Institute of Mineralogy and Crystallography "Acad. Iv. Kostov" (Bulgarian Academy of Sciences/IMC**) for the position of "professor" in the professional field 4.4. Earth Sciences.

The fulfilment of the minimum national requirements in professional field 4.4. Earth Sciences/4.2 Chemical Sciences by points is presented in the following table.

Indicators by group	Indicators	Doctor		Required points for AD "professor" by groups for 4.4. Earth Sciences		Achieved points of the candidate
		Min. requirements	Achieved points	HIPC*	BAS/IMC**	BAS/IMC**
A	1. Dissertation for the award of educational and scientific degree "Doctor"	50	50	50	50	50.00
B	3. Habilitation work - scientific publications in publications that are refereed and indexed in WoS and Scopus			100	100	112.74
Г	7. Scientific publications in journals that are refereed and indexed in WoS and Scopus, outside the habilitation thesis	30	50	200	220	236.54
Д	11. Citations in scientific publications, monographs, collective volumes and patents, refereed and indexed in WoS and Scopus			100	120	500.00
E	12. Sum of indicators from 12 to the end			150	150	350.00
	Total	80	100	600	640	1199.28

* The Law on the Development of Academic Staff in the Republic of Bulgaria

** Regulations for the conditions and procedure for the acquisition of scientific degrees and for the occupation of academic positions in the Bulgarian Academy of Sciences / Regulations for the conditions and procedure for the acquisition of scientific degrees and for the occupation of academic positions in the IMC-BAS

The made reference reveals that the scientific production of Dr. Titorenkova defends and exceeds in all indicators the increased requirements of BAS/IMC in the individual groups of indicators for scientific direction 4.4. Earth Sciences, as specified in the BAS-PRASRB and the IMK-BAS-PRASRB. These data prove that Assoc. Prof. Titorenkova is an outstanding scientist in the field with proven international prestige of research in the field of spectroscopic studies and characterization of physicochemical and crystal-chemical properties of materials.

3. Main scientific and/or applied contributions

The contributory nature of the publications with which the candidate participates in the competition has been considered in the two main categories of material according to the requirements of Article 2b, paragraphs 2 and 3 of the HRAADB: criterion "B" - Habilitation author's statement on the contributory nature of the publications, which are included in the Habilitation thesis and category "G" - Author's statement on the contributory nature of the publications by indicator. The candidate

Assoc. P. Titorenkova has presented her contributions on the publications jointly for the groups of indicators "C" and "D" in one general reference. In defence of the requirements for indicator C, Assoc. Titorenkova includes 10 publications (No. 1-10), which have been published in refereed and indexed in world-known databases of scientific information, 8 of them are in quartile Q1 and 2 publications with Q2. For the group of indicators "D", 17 publications are included in subgroup D.7 - Refereed publications (Nos. 11-27), 7 publications in subgroup G.8 - Non-refereed publications (Nos. 28-34) and in subgroup G.9 - 2 book chapters (Nos. 35, 36).

4.1. Summary of publications submitted

The scientific activity of Assoc. Titorenkova is related research in several scientific areas of synthesis and characterization of structural-phase and physicochemical properties of natural, synthetic and modified groups of materials such as 1. Biominerals and synthetic biomaterials; 2. Synthetic heteropolyhedral, porous materials; 3. Ceramics and ceramic pigments; 4. Synthetic materials; 5. Natural minerals and natural pigments; 6. Spectrophotometric methods.

4.2 Scientific contributions

The main scientific contributions in the publications of Assoc. Titorenkova can be presented in several categories:

- Gain new data on the chemical and phase composition, isomorphic substitution events, structural and crystal chemical characteristics and properties of biological, synthetic and natural minerals;

- Application of local vibrational spectroscopy methods in mineralogy for the study of biological, synthetic and natural minerals and materials;

- Establish relationships between structural characteristics, isomorphic substitution, defects and properties of minerals and materials.

The scientific contributions of Assoc. P. Titorenkova in these studies are briefly presented within the defined thematic groups.

4.2.1. Studies of biological minerals and synthetic biomaterials (B1, 2, 3, 4, 5, 6; D28 and G35)

The publications in this group deal with the synthesis of various calcium phosphates with applications in dentistry (B2, 3, 6 and G35), the influence of conditions, pH of the medium (B3, B6, G35), methods of influence and intensification on the phase composition (B2) and phase transformations in simulated media to study the degree of influence on the final products or modification of their structure (B1-6, G28, G35).

The preparation of synthetic Ca-phosphates was investigated by a biomimetic approach, i.e., in a simulated medium of tissue fluids (SBF) that differ in HCO_3^- , Cl^- ions and amino acid (glycine) content in order to mimic the biological mineralization of solid tissues. These syntheses yield amorphous dicalcium phosphate dihydrate (an analogue of the mineral brushite), which is considered to be a precursor of biological apatite that makes up mineralized tissues. Depending on the composition of the system, pH and Ca/P ratio, and residence time in different tissue fluids, dicalcium phosphate dihydrate is transformed into octacalcium phosphate (intermediate phase) and ultimately B-type carbonate-apatite at different rates (B3).

The effect of amino acid additions of glycine, alanine and valine on the biomimetic precipitation of amorphous, Mg- and Zn-doped, double-doped calcium phosphates, which after calcination are transformed into Mg, Zn- β -tricalcium phosphate (β -TCP; an analogue of the mineral vitlocite), was investigated. The influence of amino acid type and concentration on the extent of magnesium and zinc incorporation into the solid phases formed was refined by a suite of methods. Mg^{2+} and Zn^{2+} have been shown to substitute for Ca^{2+} only at the octahedral positions in the tricalcium phosphate (β -TCP) structure, and the resulting isomorphically substituted Mg,Zn- β -TCP

can serve as a reservoir for magnesium and zinc ions, in biomaterials for solid tissue remodeling (B6).

Publication B35 (book chapter) is devoted to the biomimetic precipitation and transformation of calcium ortho-phosphates. The work reviews the classification of calcium ortho-phosphates, their crystal structure, degree of solubility, review of composition, pH of electrolyte systems and their advantages. Results of biomimetic precipitation in modified SBF of different composition, biomimetic precipitation and transformation of amorphous calcium phosphate and dicalcium phosphate dihydrate, high temperature modification of ion-modified amorphous calcium phosphate into apatite are presented.

In Publication B1, the changes of dental apatite treated with different parameters of a dental pulsed Er-YAG laser ($\lambda = 2940$ nm) were investigated. The structural changes were determined by micro-infrared spectroscopy in reflection mode and Raman spectroscopy with an ultraviolet source of the excitation radiation (325 nm). Based on statistical analysis of the spectral parameters (position, width, integral intensity of the peaks generated by different atomic groups (PO_4 , CO_3 , OH and amino groups)), it was found that the effect of the dental laser was strongest on organic molecules and carbonate groups at a dental laser power of 8W. The contribution of these studies is the determination of safe parameters for dental laser operation, at which there is no disruption of the structural state of biological apatite, mobilization of carbonate and amino groups (B1).

Publications B4 and B5 present results of testing new materials for remineralization of dental apatite. The feasibility of using microgels of polymers PDMAEMA/Carbomer 940 (B4) and in the presence of polycarboxybetaine (PCB) or polysulfobetaine (PSB) (B5) to form a thin surface layer on laboratory demineralized enamel surfaces is investigated. The results demonstrate that the polymer forms spherical particles around which calcium phosphates are deposited in-situ, as demonstrated by micro-infrared, Raman spectroscopy and NMR analyses.

I will not consider publication B2 as I am a member of the author collective.

4.2.2 Synthetic heteropolyhedral porous materials - Group B7, 8, 9 and Group G19 publications

In this group of publications, we present the results of preparation and characterization of new, synthetic heteropolyhedral porous silicates. The heteropolyhedral compounds have a crystalline structure composed of silicon-oxygen tetrahedra linked by coordination polyhedra (octahedra) formed from other metals (copper, iron, titanium, zircon, etc.). Their skeletal structure resembles zeolites and zeolite-like minerals. Paper C7 presents the results of the synthesis and characterization of a new, ferrous, microporous silicate (MS-1 - $\text{Na}_{6.7} \text{Ca}_{1.3} \text{FeSi O}_{618}$) with a three-dimensional structure, analogous to the mineral imundrite of the Lovozerite group; B8 characterizes a new, indium analogue (MS-2) of the mineral imundrite ($\text{Na}_6 \text{Ca}_{1.5} \text{FeSi O}_{618}$) of the Lovozerite group, which instead of iron has a skeleton composed of $[\text{InO}_6]$ indium octahedra connected by 6-membered rings of $[\text{Si O}_{618}]$ tetrahedra; B9 presents results from three copper heteropolyhedral silicates obtained and studied: $\text{Na K}_{0.170} 8[\text{Na}_4 \text{Cu}_2 \text{Si O}_{1228} (\text{OH})(\text{H}_2 \text{O})_2 .4\text{H}_2 \text{O}_2$ (MS-3A), $\text{Na K}_{1.081.14} \text{Cu}_2 \text{Si O}_{1229} (\text{H}_2 \text{O})_2 .3.5\text{H}_2 \text{O}_2$ (MS-3B) and $\text{Na}_{1.43} [\text{Na}_4 \text{Cu}_2 \text{Si O}_{1229} (\text{H}_2 \text{O})_{2.3} .9\text{H}_2 \text{O}$ (MS-3C) and the exchanged forms Cs-MS-3A, Sr-MS-3A by hydrothermal synthesis. The materials have been studied by a complex of methods and the crystal structure, chemical composition, thermal properties have been determined. Publication D19 presents the results of hydrothermal synthesis of another heteropolyhedral microporous material, the titanosilicate Na-GTS ($\text{Na}_4 \text{Ti O}_{44} (\text{SiO})_{43} -6\text{H}_2 \text{O}$), which is a structural analog of the mineral pharmacosiderite. Its ion exchange capacity when exchanged with cobalt was investigated, and the experiments were conducted at Yamaguchi University, Japan.

4.2.3. Ceramic pigments - publications from group B10 and group G11, 12, 13, 14, 15, 29-33

In this group of publications, research has been conducted on the preparation and characterization of ceramics and ceramic pigments as part of a theme developed jointly with the University of Rousse in Razgrad and aimed at the preparation of ceramic pigments for use in sanitary ceramics. The aim of these studies is the synthesis of coloured ceramics based on pyroxene matrix (mainly from the series of solid solutions diopside-hedenbergite, diopside-enstatite and augite), by incorporating transition elements-chromophores (Co^{2+} , Mn^{2+} , Cr^{3+} , Fe^{2+} , Fe^{3+} , V^{5+} , REE^{3+}) into the structure of pyroxenes. The color of the materials is associated with the presence of transition metals incorporated in the crystal structure, which have unfilled d- or f- electron orbitals that determine the electronic transition under the action of light. The syntheses were carried out by two methods: by solid-phase high-temperature synthesis and by sol-gel method and subsequent heating at high temperatures.

The scientific contribution in these publications is related to the identification of the compositions and synthesis parameters at which ceramics are expected to form, mainly from pyroxene, so as to establish the influence of isomorphic substitution on the phase, structural and optical characteristics and on the colour of the ceramics.

4.2.4. Other synthetic materials - Publications in groups G16, 17, 18, 20, 21

This group of publications presents research on other synthetic materials with different potential applications.

In publication G16, experiments were carried out to produce a “geopolymer” by activating waste slag from the Aurubis plant (Pirdop, Bulgaria) with a phosphoric acid solution.

In Publication 17, glass is obtained in a new quaternary tellurium system TeO_2 - Bi_2O_3 - GeO_2 - Li_2O . Raman spectroscopy was used to evaluate the contributions of the different TeO_n structural units. The spectra in different polarization differ, which is an indication of the presence of unbound oxygen atoms.

Nanosized TiO_2 materials with silver-added Ag are promising photocatalysts. In Publication D18, results of preparation of TiO_2 nanosized sheets and TiO_2 thin films decorated with Ag nanoparticles by cryoliophilization and ArF laser ablation methods are presented. These materials are mainly characterized by TEM.

Publication D20 presents the results of the synthesis, crystal structure determination, thermal and spectral characterization of three Mg(II) perhenate complexes: $\text{Mg}(\text{H}_2\text{O})_2(\text{ReO})_4$ (1) and two new ionic complexes with urea ($\text{OC}(\text{NH})_2$, (U)), $[\text{Mg}(\text{H}_2\text{O})_2(\text{U})_4](\text{ReO})_4$ (2) and $[\text{Mg}(\text{U})_6](\text{ReO})_4$ (3). A detailed analysis of the vibrational and optical spectra is presented, and the density of states is performed with theoretical, periodic PAW/PBE calculations.

In Publication D21, the crystal structures of three complex compounds, magnesium iodides with urea, were determined. The studied compounds were found to crystallize in the same spacegroup $P2_1/c$ and exhibit a structure isotypic of the corresponding chlorides and bromides. The complexes have been characterized by experimental IR spectroscopic and TG-DTA analyses and DFT/B3LYP theoretical calculations of free energy and vibrational states at the molecular level.

The contribution of Assoc. Titorenkova in these studies is in the characterization of materials and obtaining new information on the structural characteristics of materials.

4.2.5. Natural minerals and natural pigments and Spectrophotometric methods - Publications of group D22, 23, 24, 25; 34, 36

Contributions to natural mineral research include the results of the description and characterization of new mineral finds of fluornavellite $\text{G22 Al}_{2.90}(\text{PO})_{42}(\text{OH})_2 \cdot [\text{F}_{0.88}(\text{OH})_{0.12}]5\text{H}_2\text{O} (+0.1\text{H}^+)$ from the Balkan Peninsula (Northern Macedonia) and Libetenite - $\text{G23 Cu}_2(\text{PO}_4)(\text{OH})$,

from the Kladenche deposit, Rosen ore field, Eastern Middle Mountains. Results include mineralogical description and data on crystal morphology, chemical composition, crystal structure and infrared spectra.

Publications G24, G25 and G34 present the results of mineralogical characterization of ancient plasters and pigments from the Early Hellenistic tomb of Dokumaci (4-3 BC), located near the town of Mangalia, Romania. The phase compositions of the plasters and pigments used for decoration were determined by optical microscopy, electron microscopy, powder X-ray phase analysis, infrared and Raman spectroscopy. In paper G36, spectral characteristics from micro-infrared and Raman spectroscopy of natural minerals used as pigments for red, black, yellow and green colour in some selected Thracian tombs in Bulgaria are presented in summary form. Contributions include spectroscopic data for specifying the composition and features of the ancient, natural pigments used.

4. Personal impressions

I know Assoc. P. I have excellent impressions of her as a dedicated scientist and researcher with high expertise in spectroscopic methods, organizational skills and experience in project initiatives. This allowed me to build a good personal and professional relationship with Assoc. Titorenkova, whom I consider to be a cordial and helpful colleague.

5. Evaluation of the personal contribution of Assoc. P. Titorenkova in the materials for the AD “Professor” competition

The thorough review of the presented scientific papers and scientific documentation gives me reason to assume that the personal contribution of Assoc. Titorenkova consistently covers all stages of scientific activity - from participation in the planning of the syntheses of various natural and synthetic samples, successively through the conduct of the analytical measurements by powder X-ray diffraction method, infrared spectroscopy, Raman, optical spectroscopy and other analytical methods, interpretation of the results and forming the publications. The active publication activity, citation rate, national and international project activity are reflected in the values of the scientific metrics, which significantly exceed the minimum national requirements of the Law on Research and Development and of the Regulations on Research and Development in the Institute of Medical Sciences-BAS for obtaining the AD "Professor" in the professional field 4.4. Earth Sciences.

6. Critical comments and recommendations

I have no critical remarks and recommendations.

7. Conclusion

The documentation submitted by Assoc. Prof. Dr. Rositsa Hristova Titorenkova for participation in the competition for the position of AD "Professor" meets the requirements of the IMC-BAS Law and the Regulations of the IMC-BAS. The evidence meets 1199.28 points and exceeds the minimum requirements under the regulations.

I positively evaluate the materials presented in the competition and recommend the Scientific Jury to propose to the Scientific Council of IMC-BAS the candidate Assoc. Prof. Dr. Rositsa Hristova Titorenkova to be elected to the academic position of "Professor" at IMC-BAS in the professional field 4.4. Earth Sciences (Mineralogy and Crystallography) for the needs of the department “Structural Crystallography and Materials Science” at the Institute of Mineralogy and Crystallography “Acad. Iv. Kostov” (IMC) - BAS.

22.03.2024
Sofia

(Prof. Dr. V. Petkova)