

## PhD thesis Review Summary

Thesis author: **Michaela Fecková**

Thesis title: **Organic and organometallic heterocyclic luminescent materials: towards OLED applications**

The aim of the dissertation work is divided into three points. The first one was to perform literature search on the subject of the dissertation work, which was done in well-written and intelligible Chapters I and II. In Chapter I, the physical basics of the absorption and emission characteristics are described in detail. A large part of this chapter is also devoted to the structure-luminescence relationship; the author describes how the size and character of the pi conjugated systems is related to their luminescence properties. The second part of this chapter describes the application of the studied materials, especially in organic light emitting diodes and organic semiconductors.

Chapter II contains description of pyrimidine-derived luminescent materials based on push-pull molecules with pyrimidine as an electron-withdrawing part of the molecule. A list of photoluminescent (PL) compounds derived from pyrimidine is presented, influence of peripheral donating groups, influence of the pi system present in this compounds – its length and character - and influence of branching are discussed. General approach to pyrimidine compounds synthesis is described. In the last part of this chapter, categorization of OLEDs, their classification into three generations and history of their development is given, with a very detailed description of pyrimidine-based 3rd-generation OLED materials. The 3rd generation is the most advantageous, employing the positive properties of both 1st and 2nd generations – light stability, high efficiency, no metal content, and production of deep-blue light. This part of the text is very detailed and illustrates very rich chemistry connected with this topic.

Chapters I and II demonstrate quite extensive theoretical part of the dissertation work with more than 200 references, which testifies the very thorough work with literature and indicate the deep knowledge the author has about the subject of the dissertation work.

Chapters III to V represent the own work of the author. All these three chapters are structured similarly. Each chapter has its own Introduction part devoted to the theoretical background of the specific problem solved in the corresponding chapter. The Introduction is then followed by a Synthesis part and parts describing X-ray analysis and thermal properties. In Chapter III this X-ray analysis and thermal properties are merged into one subchapter – I am not sure why; this should be explained by the author. Also, the term “X-ray properties” in Chapter III is not chosen very appropriately, in my opinion.

Chapter III describes arylvinylpyrimidine compounds which author synthesized and for which she studied their PL properties. Among them, the tripodal compounds (there are altogether 19 of them) are the most extensive group of the compounds she prepared and studied their solvatochromism, effect of protonation, and branching effect. The most interesting properties described for these compounds in this chapter is their two-photon absorption. It was found that for one-branched chromophores the two-photon absorption spectra are almost identical with their one-photon spectra. On the other hand, for two- and three-branched derivatives the two-photon spectra show a blue shift of their maxima compared to their one-photon spectra. The author also discusses the difference between the optical properties of these pyrimidine derived chromophores and of chromophores having a C3 symmetry. The results

presented in Chapter III were published in three papers and, in my opinion, this is the strongest part of the dissertation work.

Chapter IV deals with phenyl(arylvinyl)pyrimidines as potential emitters for white OLED. The author managed to synthesize a series of new acridane-pyrimidine derivatives. Three of them were prepared in a crystalline form suitable for single-crystal X-ray analysis and for determination of their structure. The author also characterized the final compounds from the point of view of their photophysical properties, which were discussed regarding the character of the peripheral functional groups. Altogether, six new chromophores with central pyrimidine and peripheral acridan moiety were prepared and their spectral properties were measured and discussed in connection with DFT calculations.

A little bit different type of compounds was studied in Chapter V, that is platinum complexes with phenylpyrimidine ligands. According to the author, this work was based on the work of Cao et al. The author refers to compound 227, which should be drawn in Figure 80, but is not indicated there. It is supposed that compounds of this type have promising electroluminescent properties. The author prepared five of these compounds, all of them showing strong emission in solid state. The work described in this chapter resulted in a preparation of one paper, which has been published recently in European Journal of Inorganic Chemistry.

The work of the author is intelligibly and clearly summarized in the chapter with caption "General Conclusion and perspectives". As for the title, I expected that the perspective of these materials and possible future studies in this field would be discussed more broadly.

The results of the thesis are relevant to current needs of the scientific community and of industry practice and are important for the further development in the field of lighting devices based on organic materials. This doctoral work has a strong potential as the basis for next discoveries and for its utilization in an academic field. The thesis also provided valuable evaluation of the photoluminescence properties of pyrimidine-based luminophores.

The style of the thesis is professionally cultivated, relevant and formally correct. It is a well-written work, which can be easily read and understood. Thanks to the structuring of the work, the reader is well lead through the text; all the problems regarding the subjects studied in the work are clearly explained in Chapters I and II and in the introduction parts of Chapters III to V.

The student is an author or co-author of five paper in prestigious scientific journal and assisted in writing another three papers, topics of which were quite close to the subject of the presented dissertation work. The amount of work done by the author during her PhD study, as it is presented in this Doctoral thesis and in her scientific publications, is substantial and entirely fulfils the range envisaged for such a doctoral project. As follows from the presented work, the author is very well oriented in this field of chemistry and is capable of independent scientific work, as evidenced by her publications in respected international journals.

In my opinion the thesis of Ms. **Michaela Fecková** meets all the requirements set for the dissertation works.

I therefore **recommend** the thesis for the defense.

Pardubice, 24th May 2021

  
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