Review on the PhD. thesis

Advanced Materials For Organic Photonics

elaborated by

D.E.A. Imad Ouzzane

The reviewed PhD thesis is devoted to the development of low molecular weight organic materials, i.e. diphenyl-diketo-pyrrolopyrrole (DPP) derivatives used earlier as dyes. This thesis represents a part of the complex research performed at the Faculty of Chemistry, Material Research Centre in Brno. The author presents very interesting and current material research problem connected with the development of novel organic compounds with the potential application in the optoelectronic. The obtained results may be interesting from several points of view.

The PhD thesis is logically structured into chapters and subchapters. Formally, the main part of the PhD thesis consists of five chapters, list of references and the annex part. Supplement contains five published works. The thesis is written on 122 pages altogether, and enriched by number of figures, schemes and chemical reactions (44), equations (4) and tables (6). The theoretical principles, as well as the research part, were validated with 118 valuable references. The theoretical part covers the first three chapters. They introduce the studied problems and explain the basic features and necessary notations. In Chapter 2, the state of the art is presented and a survey of methods and their brief analysis is made. The experimental part is presented in Chapter 3. The fundamental part of the PhD thesis can be found in Chapters 4 and 5 where obtained results are presented. In this context, I have several critical remarks connected with the extent of the introduction chapters and their ideological content. I suppose that the detailed explanation of employed spectroscopic techniques and terminology, which are available in many textbooks of physical chemistry and spectroscopy, is not necessary. Therefore, the subchapters 2.4 and 3.3 could be presented in shortened form. On the other hand, the detailed description and characterisation of the developed DPP molecules is missing from the chemical and syntheses procedures point of view. Next, the quantum chemistry represents very effective and useful tool enabling the interpretation of molecular electronic structure and their spectroscopic properties. Unfortunately, the PhD thesis does not contain at least minimal description of the calculation methods. I note that the shape of molecular orbitals and certain theoretical results are presented in Chapter 4. For the better understanding of the general aims of this thesis, the author could prepare the special Chapter, Aims of the PhD thesis, where the all main and partial goals of his research would be clearly listed. In the case of the Chapters 4 and 5, the personal research contribution of D.E.A. Imad Ouzzane and the main results published in the attached manuscripts could be also outlined. Finally, the conclusion part does not contain a clear summary of the planned aims and the vision of the next possible development of the DPP derivatives. The text contains several misprints or physical inconsistencies. For example, the found errors are: page 11, I have also ... (author's plural should be used); page 17, Figure 8 (is this figure completed?); the decimal points should be used instead of decimal commas (see e.g. Tables 5, 6, 8); page 45, Table 4 (Stokes' shift
should be presented in cm\(^{-1}\) – it is the energy difference); page 45, Table 4 – the error for the lifetime of compound IV is missing; pages 47 and 48, Figures 31 and 32 – are the physical units for \( P \) quantity correct?; page 64 ... of the Carbonyl ...; page 67, Figure 43, the description of the right \( y \)-axis overlapped the scale; page 79, stock shift; the references 8, 46, 74, 104 are not complete or they have the improper format.

For the better understanding of presented results, I have these questions related to the PhD thesis:
1. Could author summarise the main and partial aims of this PhD thesis?
2. Which quantum chemical methods and basis sets were used for the interpretation of the spectroscopic experiments? How the possible molecular conformations were identified?
3. Which method, basis set was used for the visualisation of the molecular orbitals presented on page 63. Which isosurface is depicted?
4. The organic materials suitable for the application in optoelectronics should possess certain electrochemical properties with respect to the anodic oxidation or cathodic reduction. Next, the molecular stability after large number of charging steps is also very important. What is the behaviour of DPP derivatives with respect to this fact?
5. Could author quantify what is his dominant contribution in the publications attached in the Supplement?
6. What is the physical meaning of the reorganisation energy? (page 63)
7. Which scientific aims were fulfilled and which not?

Despite my critical comments, D.E.A. Imad Ouzzane has proved to be capable of solving chemical research problems. His doctoral thesis presents new results of scientific relevance. Mr. Ouzzane is co-author on five publications in the international scientific journals and all of them are directly related to his PhD topic. He presented 18 oral presentations or posters on local and international conferences. In principle, the prepared structures can be used as the starting molecular series for the development of the compounds with potential usage in the optoelectronics.

The PhD thesis satisfies the conditions of the Czech Act 111/1998 and its Section 47 and therefore

I recommend

D.E.A. Imad Ouzzane’s thesis to be accepted by the Committee to be presented and defend in the branch of Chemistry, Technology and Material Properties (P2820)

Bratislava, 9\(^{th}\) January 2015

Prof. Ing. Vladimír Lukeš, DrSc.