Review of the diploma work entitled "Teoretické studium rutheniových komplexů s protinádorovými účinky/Theoretical studies of the ruthenium complexes with anti-cancer activities" by Zdeněk Futera

The diploma work of Zdeněk Futera provides a comprehensive study of the geometry and stability of the piano-chair ruthenium complexes, which are an important class of the recently discovered anticancer cisplatin-analogue drug candidates.

In this study a broad repertoire of state-of-the-art computational methods is applied to get an insight into the atomic level properties of this very interesting group of compounds. This diploma work convincingly demonstrates that the candidate mastered all basic tools used in bio-inorganic computational studies. The documented results are of scientific value and hopefully will be published in some highly impacted international journal. I am sure that they will provide a great addition to the currently available computational chemistry literature on these compounds.

The work begins with an introduction, providing an overview of the current state of the research of organometallic anticancer compounds with a special emphasize on those of ruthenium. The next part gives an insight into the theoretical basis of the computational methods applied in the forthcoming sections. This is followed by a brief description of the technical details of the calculations performed. The above three parts are well-written and show the candidate's competency in the field. In the Results part, after a detailed characterization of the basic piano-chair complexes, the candidate examines the structure and stability of the adducts formed with nucleic acid bases both in gas-phase as well as in aqueous solution employing the COSMO dielectric continuum model to account for solvent screening. Here, I especially appreciated the effort to find a relationship between the geometry, stability and electronic properties of the studied compounds. The Results part is concluded with the technically most challenging part of the work, i.e. with description of the kinetics of (i) the hydration reaction of $[(\eta^6\text{-}C_6H_6)\text{-}Ru^{II}Cl(en)]^+$ and (ii) the substitution reactions of $[(\eta^6\text{-}C_6H_6)\text{-}Ru^{II}H_2O(en)]^{2+}$ with adenine and guanine. It was nice to see the critical view of the candidate on the activation energy of the substitution reaction between guanine and $[(\eta^6\text{-}C_6H_6)\text{-}Ru^{II}H_2O(en)]^{2+}$. The Conclusions part is well-written and demonstrates the ability of the candidate to view the computed results in a broader context, which clearly proves his potential to perform scientific research. In addition, the work contains a Supplementary Material and a List of References of appropriate length.

In summary, I think the above arguments conclusively show the candidate's eligibility to obtain the M.Sc. degree.

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