**Department of Chemistry, Faculty of Science**

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April 6, 2020

**Dear Prof. Ivan Oskar Juranić**

Thank you very much for your email on 28 March, 2020 concerning our manuscript entitled “(E)-4-(((2-amino-5-chlorophenyl)imino)methyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis" (Ms. Ref. No.:  **8693**).

I’d also like to express my appreciation to reviewers who have reviewed the manuscript and made their valuable comments. For more clarification, many changes demanded by the respectable referees have been included in the manuscript. Now, the corrected manuscript and answer to questions are being sent to you.

1. **Answers to questions:**

**Q1)** - Figure 4 - in the caption is still B3LYP - it should stay M062X in the new version. Hopefully, this is the new figure with the old caption.

- Figure S1 - the same as for Figure 4

**A1)** Captions of these figures have been corrected.

**Q2)** - page 11, line 217 - a reference to Yang et al. is not formatted and is also missing from the reference list.

**A2) The ref. 40 has been corrected.**

Q3) How can authors be sure that there is no formation of binuclear species -

[CuL2Cl2]? There is a possibility that two CuLCl, with L being NNO donor,

complexes are connected via bridging Cl ions  (e.g. Crystal Growth & Design,

2019, 19, 4810-4821; Polyhedron 2013, 57, 118−126; Polyhedron 2018, 141,

60−68; Eur. J. Inorg. Chem. 2015, (5), 882−895; Polyhedron 2019, 165,

22−30, etc.).

A3) It is possible

Q4) - I agree with the authors concerning their answer A4. However, authors

should be precise what type of calculations were done - in comp details it

is stated: “NMR chemical shifts of the HL Schiff base were predicted in

DMSO solution with…” implying PCM calculations. In the Discussion,

“The experimental chemical shifts have been recorded in DMSO solution,

while the DFT-values have been calculated for an isolated HL molecule.”

Accordingly, I believe authors did PCM calculations with DMSO, but want to

stress that this, PCM solvation model is implicit. Thus all the

intermolecular molecule-solvent interactions are absent… later they say in

line with this: “The alcoholic H5 proton can engage in intermolecular

hydrogen bonds with other HL molecules as well as the molecules of solvent.

The intermolecular interactions affect the chemical shift of the H5 atom”

I would suggest authors make these statements more precise - “isolated

HL” might be misleading, as well as “were predicted in DMSO solution.”

A4) For more clarification, These sentences have been included in the text (section 4.1.3, page 11):

The DFT-chemical shift for the H5 proton of the–CH2OH group is considerably lower than its experimental value. In this work, the implicit-solvent effects have been only considered by using the PCM model. The intermolecular interactions between two molecules of the **HL** Schiff base as well as between a **HL** molecule and molecules of the DMSO solvent have been omitted. But the experimental chemical shifts have been recorded in DMSO solution, where the alcoholic H5 proton can engage in intermolecular hydrogen bonds with the other **HL** molecules as well as the molecules of solvent. The intermolecular interactions affect the chemical shift of the H5 atom.

Q5) The English language should be improved,

A5) The text of the manuscript has been modified and the requested corrections have been included in the text.

**All of the corrections have highlighted with the blue color in the text.**

Sincerely,

S. Ali Beyramabadi