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| Book Name: | [**Recent Developments in Chemistry and Biochemistry Research**](https://www.bookpi.org/bookstore/product/recent-developments-in-chemistry-and-biochemistry-research-vol-1/) |
| Manuscript Number: | **Ms\_BPR\_4042** |
| Title of the Manuscript:  | **Spectroscopic investigation and density functional theory calculations of mercaptobenzothiazole and mercaptobenzimidazole ligands and their rhenium complexes** |
| Type of the Article | **Book Chapter** |

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| PART 1: Comments |
|  | Reviewer’s comment | Author’s Feedback *(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)* |
| **Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.** | **This work is important to the scientific community since it offers a thorough analysis of rhenium complexes with ligands for mercaptobenzothiazole and mercaptobenzimidazole, which are pertinent to uses in nuclear medicine and radiopharmaceuticals. Through the combination of density functional theory (DFT) calculations and actual spectroscopy, the study provides a thorough knowledge of the bonding, electronic, and structural properties of these complexes. Particularly for the [Re(V)O]³⁺ core, which is essential for creating cutting-edge diagnostic and therapeutic medicines, the findings provide insightful information on ligand-metal interactions. Additionally, the research may be used as a guide to create comparable transition metal complexes that may find use in industry and medicine.** |  |
| **Is the title of the article suitable?****(If not please suggest an alternative title)** | **Ok** |  |
| Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here. | **The abstract briefly mentions characterization techniques (UV-Vis, IR, NMR, etc.) but does not provide specific insights into the key findings, such as bond lengths, electronic transitions, or structural features derived from the study. Including one or two significant results would strengthen the abstract. The abstract lacks a clear statement. Explicitly mention how this research advances the understanding of rhenium complexes or their potential applications in radiopharmaceuticals. Briefly highlight the relevance of these complexes for practical applications (e.g., radiopharmaceuticals or material science) to underline their importance.** |  |
| **Is the manuscript scientifically, correct? Please write here.**  | **The manuscript appears to be scientifically correct based on the provided content and methodology. The experimental techniques, such as UV-Vis, IR, and NMR spectroscopy, thermogravimetric analysis, and elemental analysis, are well-established for characterizing metal complexes, and the application of DFT with the B3LYP functional and LANL2DZ basis set is appropriate for studying heavy transition metals like rhenium. The integration of experimental and computational data strengthens the reliability of the findings.** |  |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.****-** | **The references cited adequately support the methodology, including synthesis protocols, spectroscopic techniques, and computational approaches.** |  |
| Is the language/English quality of the article suitable for scholarly communications? | **The manuscript’s language is overall adequate for scholarly communication but requires minor corrections and stylistic adjustments to meet the highest standards for publication.** |  |
| Optional/General comments | **Including a short section or paragraph suggesting directions for future research, such as exploring other ligand systems or testing biological activity, could strengthen the manuscript's appeal.** |  |

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| **PART 2:**  |
|  | **Reviewer’s comment** | **Author’s comment *(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*** |
| **Are there ethical issues in this manuscript?**  | ***(If yes, Kindly please write down the ethical issues here in details)*** |  |

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| **Reviewer Details:** |
| **Name:** | **Job W Wafula** |
| **Department, University & Country** | **Kibabii University, Kenya** |