

Special Issue

Quantum-Chemical Modeling and Design of Chelate and Macrocyclic Metal Complexes

Message from the Guest Editor

In the last 20–25 years, metal complexes formed by chelating and macrocyclic organic and organo-element ligands (in particular, various crown ethers, cryptands, calixarenes, and porphyrins) have gained particular interest in coordination and inorganic chemistry. These compounds have a number of specific (sometimes unique) properties, due to which they have found many applications in various fields of science and in the practice of anthropogenic activities.

Original full articles and short communications devoted to quantum-chemical calculations of metal complexes of p-, d-, and f-elements, with open and closed circuits formed by organic and organo-element ligands, are preferred for this Special Issue. We welcome articles in which, along with the required quantum-chemical calculations, experimental data is presented to evaluate the reliability of these calculations. Review articles may also be submitted for publication (including author reviews, the emphasis of which is mainly on the authors' work).

Guest Editor

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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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