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**DESCRIPTION**

The *Journal of Molecular Structure* is dedicated to the publication of full-length articles and review papers, providing important **new structural information** on all types of chemical species including:

- Stable and unstable **molecules** in all types of environments (vapour, molecular beam, liquid, solution, liquid crystal, solid state, matrix-isolated, surface-absorbed etc.)
- **Chemical intermediates**
- Molecules in **excited states**
- **Biological molecules**
- **Polymers**.

The methods used may include any combination of spectroscopic and non-spectroscopic techniques, for example:

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- Optical rotatory dispersion and circular dichroism
- Fluorescence and phosphorescence techniques
- Electron spectroscopies (PES, XPS), EXAFS, etc.
- Microwave spectroscopy
- Electron diffraction
- NMR and ESR spectroscopies
- Mössbauer spectroscopy
- X-ray crystallography
- Charge Density Analyses
- Computational Studies *(supplementing experimental methods)*

We encourage publications combining theoretical and experimental approaches. **The structural insights gained by the studies should be correlated with the properties, activity and/or reactivity of the molecule under investigation and the relevance of this molecule and its implications should be discussed.**

**IMPORTANT NOTE:** Papers describing routine studies of little structural significance (e.g. manuscripts dealing only with glassy materials, characterization of particles and materials by
using microscopy techniques, those reporting essentially crystal data accompanied by routine spectroscopic studies and/or theoretical structure analysis performed for isolated molecules, and routine spectroscopy studies for commercially available compounds) are not acceptable. The same applies to manuscripts mainly focused on synthesis procedures or evaluation of bioactivity of chemical species. Solely theoretical studies should rather be submitted to Computational and Theoretical Chemistry.

AUDIENCE

Chemical Physicists, Chemists, and Biochemists, concerned with Molecular Structure and Dynamics.

IMPACT FACTOR

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INTRODUCTION

The Journal of Molecular Structure is dedicated to the publication of full-length articles and review papers, providing important new structural information on all types of chemical species including:

- stable and unstable molecules in all types of environments (vapour, molecular beam, liquid, solution, liquid crystal, solid state, matrix-isolated, surface-absorbed etc.)
- chemical intermediates
- molecules in excited states
- biochemicals
- polymers.

The methods used may include any combination of spectroscopic and non-spectroscopic techniques, for example:

- infrared spectroscopy (mid, far, near)
- Raman spectroscopy and non-linear Raman methods (CARS, etc.)
- force constant and molecular mechanics calculations
- electronic absorption spectroscopy
- optical rotatory dispersion and circular dichroism
- fluorescence and phosphorescence techniques
- electron spectroscopies (PES, XPS), EXAFS, etc.
- microwave spectroscopy
- electron diffraction
- NMR and ESR spectroscopies
- Mössbauer spectroscopy
- X-ray crystallography.

Papers describing routine studies of little structural significance (e.g. straightforward X-ray crystal structure determinations) are not encouraged.

Publications combining experimental and theoretical approaches to a problem are particularly welcomed. However, solely theoretical (semiempirical or ab initio) studies should be submitted to the Journal of Molecular Structure: THEOCHEM

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