

## Tentative Outline

### Special Thematic Issue for the journal "Current Organic Synthesis"

#### Title of the Thematic Issue: Combinatorial Study of Organic Structures

*Guest Editor: Prof. Dr. Jia-Bao Liu*

*Co-Guest Editor: Dr. Masood Ur Rehman*

- **Scope of the Thematic Issue:**

Motivation for founding graph theory has come from applications in Chemistry and Physics. One of the main applications of graph theory to Chemistry is the application in a theory of unsaturated conjugated hydrocarbons known as Hückel molecular orbital. The spectra of graphs, or the spectra of certain matrices which are closely related to adjacency matrices appear in a number of problems in quantum chemistry and statistical physics. For example, by using the eigenvalues of molecular graphs one can investigate the total pi-electron energy of molecular graphs etc.

Further it is well known that total pi-electron energy and topological indices of molecular graphs are interrelated. In fact, a topological index correlates certain physicochemical property of chemical compounds with molecular structure, such as boiling point, stability energy, and so on. It is created by converting a chemical network into a numeric quantity associated with a molecular graph, which describes the structure's topology and is an invariant understructure that preserves mappings.

This special issue aims to offer an opportunity to researchers to discuss and share their own ideas in investigating the use of graph theory in chemistry. We would like that; this special issue enables to solve some practical graph theoretic problems arises in quantum chemistry and other area of chemistry. Specially, research articles that covers the applications of graph structures and models in Chemistry, Physics and chemical engineering are welcome.

**Keywords:** Chemical graph theory, Molecular graph, Eigenvalue of molecular graph, Spectral properties of molecular graph, Energy of molecular graph, Topological index of molecular graph.

#### Sub-topics:

- Topological indices of molecular graphs.
- Bounds on topological indices for molecular graphs.
- Pi-electron energy of molecular graphs.
- Application of graph theory in chemistry.

#### Tentative titles of the articles:

- Bounds on topological indices of chemical graphs
- Laplacian energy of molecular graphs
- Graph theoretic approach to chemical structures
- Some study of molecular graphs
- Omega index of graphs
- Algebraic properties of molecular graphs
- Total pi-electron energy of hydrocarbon molecules
- Energy-like invariant of molecular graphs
- Sharp bounds on topological indices for molecular graphs
- New bounds for ABC index
- Spectral properties of chemical structures

➤ Energy and topological indices of chemical networks

#### Schedule:

✧ Thematic issue submission deadline: May 15, 2023

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