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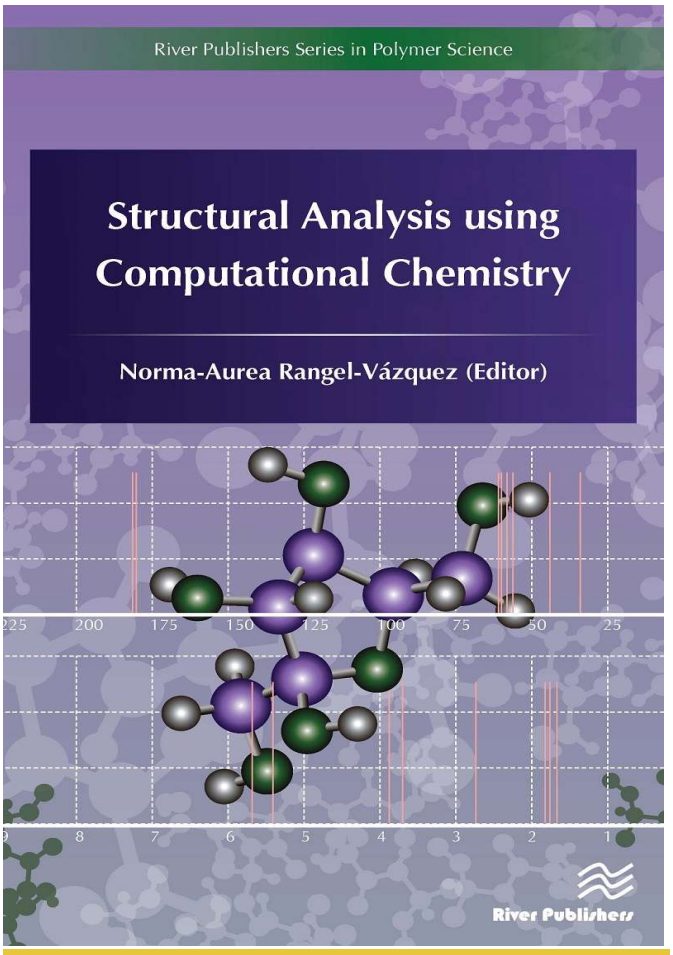
Structural Analysis using Computational Chemistry

Editor: Norma Aurea Rangel-Vázquez, PCC, Aguascalientes, México

Computational chemistry is a science that allows researchers to study, characterize and predict the structure and stability of chemical systems. In other words: studying energy differences between different states to explain spectroscopic properties and reaction mechanisms at the atomic level. This field is gaining in relevance and strength due to field applications from chemical engineering, electrical engineering, electronics, biomedicine, biology, materials science, to name but a few. *Structural Analysis using Computational Chemistry* arises from the need to present the progress of computational chemistry in various application areas.

Technical topics discussed in the book include:

- Quantum mechanics and structural molecular study (AM1)
- Application of quantum models in molecular analysis
- Molecular analysis of insulin through controlled adsorption in hydrogels based on chitosan
- Analysis and molecular characterization of organic materials for application in solar cells
- Determination of thermodynamic properties of ionic liquids through molecular simulation



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