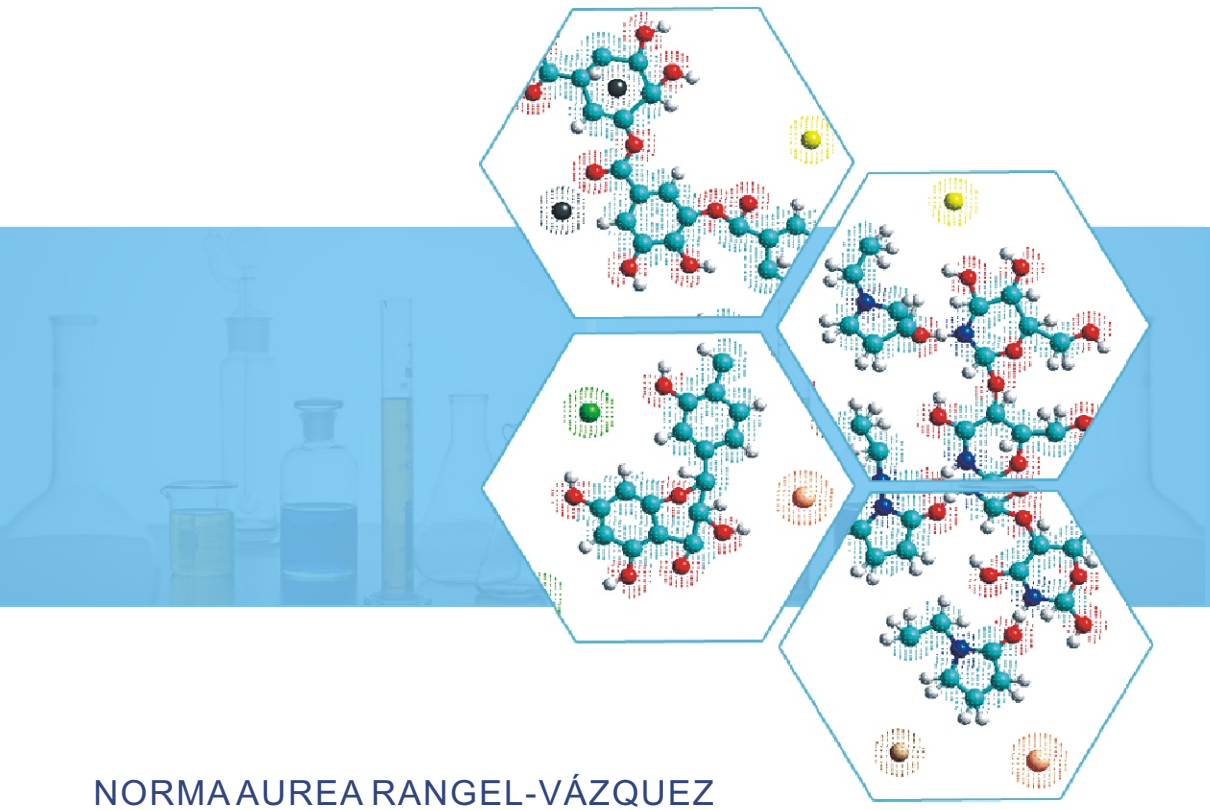
Computational Chemistry Applied in the Analyses of Chitosan/ Polyvinylpyrrolidone/ *Mimosa Tenuiflora*



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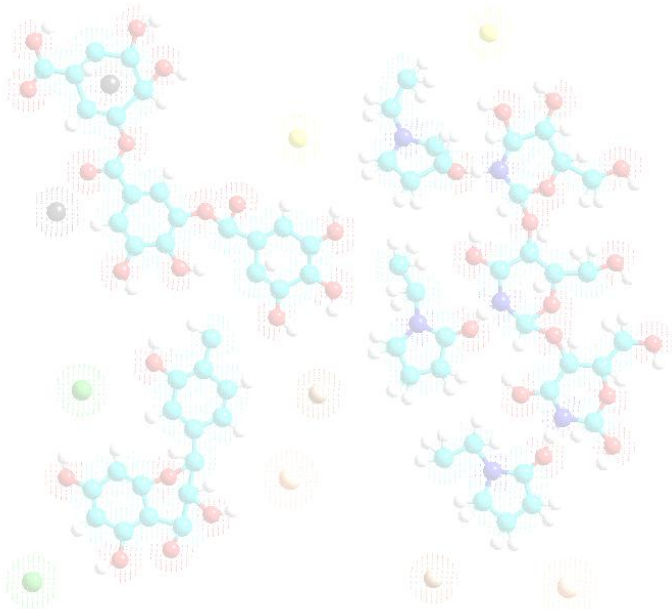

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Preface

Computational chemistry allows using various models analyze and predict the behavior of single and composite materials to determine the composition of new materials.

It should be noted that a model is a representation of the construction and working of some system of interest. A model is similar to but simpler than the system it represents. One purpose of a model is to enable the analyst to predict the effect of changes to the system. On the one hand, a model should be a close approximation to the real system and incorporate most of its salient features. On the other hand, it should not be so complex that it is impossible to understand and experiment with it. A good model is a judicious tradeoff between realism and simplicity.

This book is aimed at researchers and students with basic knowledge of computational chemistry, interested in analyzing and discussing the structural properties of different polymers. It should be noted that this book is carried out an analysis of polymers such as Chitosan, PVP and MT as well as the structure of the model from the mixture of these polymers using a computational analysis using a comparison between PM3 and AM1 semi-empirical methods, respectively.

In this case, Chitosan is a linear polysaccharide composed of randomly distributed β-(1-4)-linked D-glucosamine (deacetylated unit) and N-acetyl-D-glucosamine (acetylated unit). It is made by treating shrimp and other crustacean shells with the alkali sodium hydroxide. Chitosan has a number of commercial and possible biomedical uses. It can be used in agriculture as a seed treatment and biopesticide, helping plants to fight off fungal infections. In winemaking it can be used as a fining agent, also helping to prevent spoilage. In industry, it can be used in a self-healing polyurethane paint coating. In medicine, it may be useful in bandages to reduce bleeding and as an antibacterial agent; it can also be used to help deliver drugs through the skin.

PVP was first synthesized by Walter Reppe and a patent was filed in 1939 for one of the most interesting derivatives of acetylene chemistry. PVP was initially used as a blood plasma substitute and later in a wide variety of applications in medicine, pharmacy, cosmetics and industrial production. It is used as a binder in many pharmaceutical tablets; it simply passes through the body when taken

orally. However, autopsies have found that crospovidone does contribute to pulmonary vascular injury in substance abusers who have injected pharmaceutical tablets intended for oral consumption. The long-term effects of crospovidone within the lung are unknown. PVP added to iodine forms a complex called povidone-iodine that possesses disinfectant properties. This complex is used in various products like solutions, ointment, pessaries, liquid soaps and surgical scrubs. It is known under the trade name Betadine and Pyodine. It is used in pleurodesis (fusion of the pleura because of incessant pleural effusions). For this purpose, povidone iodine is equally effective and safe as talc, and may be preferred because of easy availability and low cost.

Finally, *Mimosa tenuiflora*, syn. *Mimosa hostilis* (Jurema, Tepezcohuite) is a perennial tree or shrub native to the northeastern region of Brazil (Para ba, Rio Grande do Norte, Cear á, Pernambuco, Bahia) and found as far north as southern Mexico (Oaxaca and coast of Chiapas). It is most often found in lower altitudes, but it can be found as high as 1000 m. *Mimosa tenuiflora* is a very good source of fuel wood and works very well for making posts, most likely because of its high tannin content (16%), which protects it from rot.

Due to its high tannin content, the bark of the tree is widely used as a natural dye and in leather production. It is used to make bridges, buildings, fences, furniture and wheels. It is an excellent source of charcoal and at least one study has been done to see why this is the case.

Finally, an important difference that has this book is, the analysis and determination of properties such as FTIR, electrostatic potentials and structural parameters of polymers in an individual way and in union, to propose a structure for a new material that has great features to be applied in the medical field and thus contribute to a need in society in general.

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