

List of Abbreviations

AIBN	Azobisisobutyronitrile
AM1	Austin model 1
AMBER	Assisted Model Building with Energy Refinement
CT	Charge transfer
ΔG	Gibbs free energy
%DD	Degree of deacetylation
eV	Electron-volt
FTIR	Fourier transform infrared spectroscopy
HOMO	Highest energy occupied molecular orbital
J	Joule
LUMO	Lowest energy occupied molecular orbital
MC	Mannosylated chitosan
MESP	Molecular electrostatic potential
MNDO	Modified Neglect of Diatomic Overlap
MT	<i>Mimosa tenuiflora</i>
NMR	Nuclear Magnetic Resonance
MO	Molecular orbital
PM3	Parametrization model 3
PPP	Pariser–Parr–Pople method
PVP	Polyvinylpyrrolidone

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

Modeling is the process of producing a model; 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.

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