



Spectroscopy and Modeling of Biomolecular Building Blocks

Jean-Pierre Schermann

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This book presents an overview of recent advances in the intertwining of the following research fields: photon and electron spectroscopy, quantum chemistry, modelling and mass-spectrometry. The coupling of these disciplines offers a new point of view to the understanding of isolated elementary building blocks of biomolecules and their assemblies. It allows the unambiguous separation between intrinsic properties of biomolecular systems and those induced by the presence of their environment.

The first chapters provide background in modelling (I), frequency-resolved spectroscopy using microwave, infrared and UV photons, time-resolved spectroscopy in the femtosecond domain and energy-resolved electron spectroscopy (II) and production of gas-phase neutral and ionic biomolecular species, mass-spectrometry, ion mobility and BIRD techniques (III).

Chapter IV is devoted to case studies of gas-phase experimental investigations coupled to quantum or classical calculations. The topics are structural studies of nucleobases and oligonucleotides, peptides and proteins, sugars; neuromolecules; non-covalent complexes; chiral systems, interactions of low-energy electrons with biomolecules in the radiation chemistry context and very large gas-phase biomolecular systems.

The fifth chapter concerns the link between gas-phase and liquid-phase. Different treatments of solvation are illustrated through examples pointing out the influence of progressive addition of water molecules upon properties of nucleobases, peptides, sugars and neuromolecules.

Offer a new perspective to the understanding of isolated elementary building blocks of bio molecules

Includes case studies of experimental investigations coupled to quantum or classical calculations

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