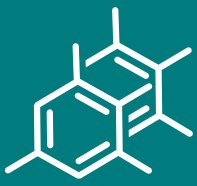

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Intramolecular Hydrogen Bonding 2021

Edited by: Mirosław Jabłoński

This book describes the results of both theoretical and experimental research on many topical issues in intramolecular hydrogen bonding. Its great advantage is that the presented research results have been obtained using many different techniques. Therefore, it is an excellent review of these methods, while showing their applicability to the current scientific issues regarding intramolecular hydrogen bonds. The experimental techniques used include X-ray diffraction, infrared and Raman spectroscopy (IR), nuclear magnetic resonance spectroscopy (NMR), nuclear quadrupole resonance spectroscopy (NQR), incoherent inelastic neutron scattering (IINS), and differential scanning calorimetry (DSC). The solvatochromic and luminescent studies are also described. On the other hand, theoretical research is based on ab initio calculations and the Car–Parrinello Molecular Dynamics (CPMD). In the latter case, a description of nuclear quantum effects (NQE) is also possible. This book also demonstrates the use of theoretical methods such as Quantum Theory of Atoms in Molecules (QTAIM), Interacting Quantum Atoms (IQA), Natural Bond Orbital (NBO), Non-Covalent Interactions (NCI) index, Molecular Tailoring Approach (MTA), and many others.

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