



COMPUTATIONAL CHEMISTRY AND SPECTROSCOPY

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Condition: New. Publisher/Verlag: VDM Verlag Dr. Müller | THEORETICAL AND SPECTROSCOPIC STUDIES ON WEAKLY BOUND COMPLEXES AND ACETYLENE | Inter/intramolecular interactions are of a major scientific interest. These interactions constitute a major part of science, ranging from material sciences to biological sciences. The chemistry of these is of fundamental importance, as they play an important role in reaction intermediates, different conformation and configuration of the molecular systems etc. In general, they contribute much towards the relative orientation of the molecules. van der Waals interactions are weak intermolecular interactions while hydrogen bonding varies in strength from weak to strong (1 to 40 kcal/mol). The present work focuses on applying some theoretical methods (ab initio and Atoms In Molecules theory) on these interactions to differentiate them with physically meaningful parameters such as hydrogen bond radii and atoms in molecules theory parameters. | Format: Paperback | Language/Sprache: english | 416 gr | 300 pp.

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