

1. Record Nr.	UNINA9910452119703321
Autore	Scheiner Steve
Titolo	Hydrogen bonding [[electronic resource]] : a theoretical perspective / / Steve Scheiner
Pubbl/distr/stampa	New York, : Oxford University Press, 1997
ISBN	1-280-52748-X 9786610527489 0-19-802509-2 1-4294-1950-4
Descrizione fisica	1 online resource (396 p.)
Collana	Topics in physical chemistry
Disciplina	541.2/26
Soggetti	Hydrogen bonding Quantum chemistry Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Contents; Abbreviations; 1 QUANTUM CHEMICAL FRAMEWORK; 2 GEOMETRIES AND ENERGETICS; 3 VIBRATIONAL SPECTRA; 4 EXTENDED REGIONS OF POTENTIAL ENERGY SURFACE; 5 COOPERATIVE PHENOMENA; 6 WEAK INTERACTIONS, IONIC H-BONDS, AND ION PAIRS; Index of Complexes; Subject Index
Sommario/riassunto	Explains the literature in which the characteristics of hydrogen bonds have been probed by quantum chemical methods. After an explanation as to how various properties are calculated, this book describes the results that have been obtained in various systems, focusing on the energetics, equilibrium geometries, and vibrational spectras.