

1. Record Nr.	UNINA9910140843103321
Autore	Allinger Norman L
Titolo	Molecular structure : understanding steric and electronic effects from molecular mechanics // Norman L. Allinger
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, c2010
ISBN	9786612707650 9781282707658 1282707655 9780470608852 0470608854 9780470608845 0470608846
Edizione	[1st ed.]
Descrizione fisica	1 online resource (355 p.)
Disciplina	547/.13
Soggetti	Molecular structure Physical organic chemistry
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 index.
Nota di contenuto	Introduction -- Experimental molecular structures -- Molecular structures by computational methods -- Molecular mechanics of alkanes -- Conjugated systems -- "Effects" in organic chemistry -- More "effects" : negative hyperconjugation -- Additional stereochemical effects in carbohydrates -- Lewis bonds -- Crystal structure calculations -- Heats of formation.
Sommario/riassunto	A guide to analyzing the structures and properties of organic molecules Until recently, the study of organic molecules has traveled down two disparate intellectual paths-the experimental, or physical, method and the computational, or theoretical, method. Working somewhat independently of each other, these disciplines have guided research for decades, but they are now being combined efficiently into one unified strategy. Molecular Structure delivers the essential fundamentals on both the experimental and computational methods, then goes further to show how these approaches can join forces to produce more effective analysis of the structure and properties of organic

compounds.
