

1. Record Nr.	UNINA9910451673103321
Autore	Rogers Donald <1932->
Titolo	Heats of hydrogenation [[electronic resource]] : experimental and computational hydrogen thermochemistry of organic compounds // Donald W. Rogers
Pubbl/distr/stampa	Singapore ; ; Hackensack, NJ, : World Scientific, c2006
ISBN	1-281-37300-1 9786611373009 981-277-290-1
Descrizione fisica	x, 222 p. : ill
Disciplina	547/.23
Soggetti	Hydrogenation Organic compounds - Thermal properties Thermochemistry Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references (p. 207-218) and index.
Nota di contenuto	Hydrogen Thermochemistry: Definition; History; Theory and Methodology; Accuracy; Applications; Details of Calorimeter Construction; Design Modifications; Experimental Results: Enthalpies of Hydrogenation; Computational Thermochemistry: Introduction to Computational Thermochemistry; Molecular Modeling; Additivity Methods; Molecular Mechanics; Molecular Orbital Calculations; Semiempirical Methods; Ab Initio Methods.
Sommario/riassunto	Heats of hydrogenation constitute a body of thermochemical information that has had an on-going significance despite the small number of research groups engaged in it. This book concentrates on the features of hydrogen thermochemistry which include historical aspects and impact of the advances in computer software on the calculation of the heats.