Record Nr. UNINA9910778262703321 Autore Rogers Donald <1932-> Titolo Heats of hydrogenation [[electronic resource]]: experimental and computational hydrogen thermochemistry of organic compounds // Donald W. Rogers Singapore;; Hackensack, NJ,: World Scientific, c2006 Pubbl/distr/stampa **ISBN** 1-281-37300-1 9786611373009 981-277-290-1 Descrizione fisica x, 222 p.: ill Disciplina 547/.23 Hydrogenation Soggetti Organic compounds - Thermal properties Thermochemistry Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Bibliographic Level Mode of Issuance: Monograph Note generali 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.