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Autore	Gavezzotti Angelo
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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	Contents; PART I: FUNDAMENTALS; 1 The molecule: structure, size and shape; 1.1 Atoms and bonds; 1.2 Classification concepts in many particle systems; 1.3 Must a molecule have a size?; 1.4 Must a molecule have a shape?; 1.5 Historical portraits: a chemistry course in the early 1960's; 2 Molecular vibrations and molecular force fields; 2.1 Vibrational modes and force constants; 2.2 Molecular mechanics; 2.3 Evolution of molecular force fields; 2.4 Appendix: an example of coordinate transformation; 2.5 Historical portraits: Got a force constant?; 3 Quantum chemistry 3.1 Some fundamentals of quantum mechanics 3.2 The hydrogen atom and atomic orbitals; 3.3 Spin; 3.4 Many-electron systems; 3.5 Molecular orbitals: The Fock and Roothaan equations; 3.6 Approximate quantum chemical methods: NDO and EHT; 3.7 Evolution of quantum chemical calculations: Beyond Hartree-Fock; 3.8 Dimerization energies

and basis set superposition error; 3.9 Historical portraits: early experiences in quantum chemistry; 4 The physical nature and the computer simulation of the intermolecular potential; 4.1 Experimental facts and conceptual framework  
4.2 The representation of the molecular charge distribution and of the electric potential 4.3 Coulombic potential energy; 4.4 Polarization (electrostatic induction) energy; 4.5 Dispersion energy; 4.6 Pauli (exchange) repulsion energy; 4.7 Total energies versus partitioned energies; 4.8 Intermolecular hydrogen bonding; 4.9 Simulation methods; 4.10 Ad hoc or transferable? Force field fitting from ab initio calculations; 5 Crystal symmetry and X-ray diffraction; 5.1 A structural view of crystal symmetry: bottom-up crystallography; 5.2 Space group symmetry and its mathematical representation  
5.3 von Laue's idea, 1912 5.4 The structure factor; 5.5 Miller indices and Bragg's law; 5.6 The electron density in a crystal; 5.7 The atomic prejudice; 5.8 Structure and X-ray diffraction: Some examples; 5.9 Historical portraits: Training of a crystallographer in the 1960's; 6 Periodic systems: Crystal orbitals and lattice dynamics; 6.1 The mathematical description of crystal periodicity; 6.2 The electronic structure of solids; 6.3 Lattice dynamics and lattice vibrations; 7 Molecular structure and macroscopic properties: Calorimetry and thermodynamics; 7.1 Molecules and macroscopic bodies  
7.2 Energy 7.3 Heat capacity; 7.4 Entropy; 7.5 Free energy and chemical equilibrium; 7.6 Thermodynamic measurements; 7.7 Derivatives; 8 Correlation studies in organic solids; 8.1 The Cambridge Structural Database (CSD) of organic crystals; 8.2 Structure correlation; 8.3 Retrieval of molecular and crystal structures from the CSD; 8.4 The SubHeat database; 8.5 The geometrical categorization of intermolecular bonding; 8.6 Space analysis of molecular packing modes; 8.7 The calculation of intermolecular energies in crystals; 8.8 General-purpose force fields for organic crystals  
8.9 Accuracy and reproducibility

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## Sommario/riassunto

The book is divided in two parts, to supply first the basic elements of the language, with short but complete explanations of terms, methods and theories; and then to describe the present status of studies on the processes by which organic molecules aggregate to form observable bodies and to determine their physical and chemical properties. - ;This book is divided in two parts. Part I provides a brief but accurate summary of all the basic ideas, theories, methods, and conspicuous results of structure analysis and molecular modelling of the condensed phases of organic compounds: quantum chemist

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2. Record Nr.	UNINA9910163203303321
Autore	duchesse d'Abrantes Laure Junot
Titolo	Memoirs Of The Emperor Napoleon - From Ajaccio To Waterloo, As Soldier, Emperor And Husband - Vol. I
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ISBN	9781782891468 1782891463
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Collana	Memoirs Of The Emperor Napoleon - From Ajaccio To Waterloo, As Soldier, Emperor And Husband ; ; v.1
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Soggetti	Napoleonic Wars, 1800-1815 Biography
Lingua di pubblicazione	Inglese
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Nota di contenuto	Intro -- TABLE OF CONTENTS -- ILLUSTRATIONS -- VOLUME I. -- VOLUME II. -- VOLUME III. -- SPECIAL INTRODUCTION -- PREFATORY REMARKS BY THE DUCHESS D'ABRANTES. -- THE AUTHOR'S INTRODUCTION TO THE ORIGINAL EDITION. -- CHAPTER I. -- Place and Date of My Birth-Calomeros and Bonaparte-My Father's Departure for America-Intimacy between My Mother and Madame Letitia- Bonaparte's Boyhood - The Basket of Grapes and the Flogging - Saveria and the Bonaparte Family - My Father's Return-My Birth and My Mother's Illness. -- CHAPTER II. -- My Mother's Drawing-room-The Comtesse de Perigord-The Duchesse de Mailly and the Prince de Chalais -Louis XV. and the Comtesse de Perigord -The Duchesse de Mailly and the Princesse de Lamballe- Bonaparte's First Arrival in Paris- His Intention of Presenting His Character when a Young Man. -- CHAPTER III. -- Death of Bonaparte's Father in My Mother's House-Joseph Bonaparte and M. Fesch - Removal of My Family to Paris - M. de Saint Priest, M. Segurier, and M. Duvidal de Montferrier -Madame de Lamarliere-A Wedding Feast at Robespierre's-The Queen at the ConciergerieMM. d'Aigrefeuille and Cambaceres. -- CHAPTER IV. -- Marianne Bonaparte at Saint Cyr-Humbled Pride- Bonaparte Made Sub-Lieutenant - His First Appearance

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Lucien in Danger, and His Deliverance-Hopes Created by the Chief of the Consular Government-Lucien Minister of the Interior -Scene at Malmaison, and Conversation with the First Consul.

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Sommario/riassunto

This book, originally published in 1901, is a memoir by Madame Junot, Duchess D'Abrantès, detailing the life of Napoleon Bonaparte from his early years in Ajaccio to his final battle at Waterloo. The memoir offers a personal and detailed account of Napoleon's life, exploring his roles as a soldier, emperor, and husband. It provides insights into his character, ambitions, and relationships, as observed by the author who was closely associated with him. The narrative captures the tumultuous period of the late 18th and early 19th centuries, marked by revolutionary upheaval and political intrigue. Intended for readers interested in historical biographies and the Napoleonic era, the book combines personal anecdotes with historical events, offering a unique perspective on one of history's most iconic figures.

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