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Autore	Coppens Philip
Titolo	X-ray charge densities and chemical bonding [[electronic resource] /] / Philip Coppens
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Nota di contenuto	Contents; Chapter 1 Scattering of X-rays and Neutrons; Chapter 2 The Effect of Thermal Vibrations on the Intensities of the Diffracted Beams; Chapter 3 Chemical Bonding and the X-ray Scattering Formalism; Chapter 4 Least-Squares Methods and Their Use in Charge Density Analysis; Chapter 5 Fourier Methods and Maximum Entropy Enhancement; Chapter 6 Space Partitioning and Topological Analysis of the Total Charge Density; Chapter 7 The Electrostatic Moments of a Charge Distribution; Chapter 8 X-ray Diffraction and the Electrostatic Potential Chapter 9 The Electron Density and the Lattice Energy of Crystals Chapter 10 Charge Density Studies of Transition Metal Compounds; Chapter 11 The Charge Density in Extended Solids; Chapter 12 Electron Density Studies of Molecular Crystals; Appendix A: Tensor Notation; Appendix B: Symmetry and Symmetry Restrictions; Appendix C: The 50% Probability Ellipsoid; Appendix D: Spherical Harmonic Functions; Appendix E: Products of Spherical Harmonic

Functions; Appendix F: Energy-Optimized Single- Slater Values for Subshells of Isolated Atoms; Appendix G: Fourier-Bessel Transforms Appendix H: Evaluation of the Integrals $A_{[sub(N)], [sub(l)][sub(1)] [sub(l) [sub(2)] [sub(k)](Z, R)}$ Occurring in the Expression for the Peripheral Contribution to the Electrostatic Properties Appendix I: The Matrix $M [sup(-1)]$ Relating d-Orbital Occupancies $P [sub(ij)]$ to Multipole Populations $P [sub(lmp)]$; Appendix J: The Interaction Between Two Nonoverlapping Charge Distributions; Appendix K: Conversion Factors; Appendix L: Selected Exercises; References; Index

Sommario/riassunto

This book deals with the electron density distribution in molecules and solids as obtained experimentally by X-ray diffraction. It is a comprehensive treatment of the methods involved, and the interpretation of the experimental results in terms of chemical bonding and intermolecular interactions. Inorganic and organic solids as well as metals are covered in the chapters dealing with specific systems.

2. Record Nr.	UNINA9910446326203321
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Contents; Contributors; Jack Hawkes: Plant Collector, Researcher, Mentor and Visionary; Preface; Foreword; Acknowledgements; Part I:

Crop Wild Relative Conservation and Use: an Overview; Part II: Establishing Inventories and Conservation Priorities; Part III: Threat and Conservation Assessment; Part IV: Genetic Erosion and Genetic Pollution; Part V: In Situ Conservation; Part VI: Ex Situ Conservation; Part VII: Information Management; Part VIII: Gene Donors for Crop Improvement; Part IX: Use of Crop Wild Relatives and Underutilized Species
Part X: Global Issues in Crop Wild Relative Conservation and UseIndex

Sommario/riassunto

Crop wild relatives (CWR) are species closely related to crop plants which can contribute beneficial traits such as pest or disease resistance and yield improvement. Through an examination of national, regional and global context of CWR, this text presents methodologies and case studies that provide recommendations for global conservation and use.
