

1. Record Nr.	UNINA9910450681603321
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Titolo	X-ray charge densities and chemical bonding [[electronic resource] /] / Philip Coppens
Pubbl/distr/stampa	[Chester, England], : International Union of Crystallography ; Oxford New York, : Oxford University Press, 1997
ISBN	0-19-756087-3 1-280-52811-7 9786610528110 0-19-535694-2 1-4294-1461-8
Descrizione fisica	1 online resource (373 p.)
Collana	International Union of Crystallography texts on crystallography ; ; 4
Disciplina	548/.3
Soggetti	X-ray crystallography Chemical bonds Electron distribution Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Previously issued in print: 1997.
Nota di bibliografia	Includes bibliographical references (p. 328-346) and index.
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 $M^{[-1]}$ 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.
