

Electron density and chemical bonding II : theoretical charge density studies

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Abstrak

This book about new directions in pseudoatom-based X-ray charge density analysis, reliable measurements of dipole moments from single-crystal diffraction data and assessment of an in-crystal enhancement, challenging problems in charge density determination : polar bonds and influence of the environment, electron density in quantum theory, residual density analysis, the source function descriptor as a tool to extract chemical information from theoretical and experimental electron densities.