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Collana	Chemistry research and applications
Altri autori (Persone)	PutzMihai V
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Livello bibliografico	Monografia
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	<p>""1. Why a Reappraisal Is Necessary """"2. The Relevance of the Classical Framework ""; ""3. On the Two Kinds of Incompatibility ""; ""4. Wholeness and the Proper Logic for Complementarity ""; ""5. The Reduction of Duality ""; ""References ""; ""COMPLEMENTARITY OUT OF CONTEXT: ESSAY ON THE RATIONALITY OF BOHRa€?S THOUGHT""; ""Abstract ""; ""1. Complementarity Contextualized ""; ""2. Complementarity: A Stumbling Block on the Way to Context ""; ""3. The Duality Route to Context ""; ""4. Incommensurability: Last Resorta€?and Last Exit ""; ""5. The Concept of Action Quantization ""</p> <p>""6. Tying Loose Ends """"Appendix ""; ""Notes ""; ""References ""; ""MOLECULAR INTEGRALS OVER SLATER-TYPE ORBITALS. FROM PIONEERS TO RECENT DEVELOPMENTS""; ""Abstract""; ""1.Introduction""; ""2.Early History of the Slater Orbitals""; ""3.History of the STO Computer Programs""; ""4.Slater Orbitals & Gaussian Orbitals""; ""5. Types of Exponentially Decaying Orbital, Based on Eigen-functions for One-Electron Atoms""; ""6.Types of Integral over Slater Orbitals""; ""6.1. One-Electron Integrals""; ""6.2.Two-Electron Integrals""; ""6.3.Three- and Four-Electron Integrals""</p> <p>""7.Methods in the Literature""""7.1.Single-Center Expansion""; ""7.2. Gaussian Expansion""; ""7.3.Gaussian Transform Method""; ""7.4. Fourier-Transform Method""; ""7.5.Use of Sturmians""; ""7.6.Elliptic</p>

Coordinate Method"; "8.General Two-electron Exponential Type
Orbital Integrals in Poly-Atomics without Orbital Translations"; "8.1.
Introduction"; "8.2.Basis Sets"; "8.3.Programming Strategy"; "8.4.
Avoiding ETO Translations for Two-Electron Integrals over Three and
Four Centers"; "8.5.Numerical Results of Coulomb Resolutions:
Efficiency"
"8.6.Selected Exchange Integrals for the CH₃F Molecule (Evaluated
Using the Coulomb Resolution)" "8.7.Conclusions"; "9.Explicitly
Correlated Methods for Molecules"; "10.Highly Accurate Calculations
Using STOs"; "11.Closing Remarks"; "Acknowledgements";
"References"; "TUNNELING DYNAMICS AND ITS SIGNATURES IN
COUPLED SYSTEMS"; "Abstract"; "1.Introduction"; "2.Historical
Development"; "A.Tunneling in Physics"; "B.Tunneling in Chemistry";
"C.Tunneling in Coupled Systems"; "3.The Method"; "A.Dynamics of
the Coupled System in the Absence of Driving"
"B.Dynamics of the Coupled System in the Presence of External
Driving"
