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Altri autori (Persone)	PutzMihai V
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Nota di contenuto	""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 "" ""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"" ""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 Coordinate Method""; ""8.General Two-electron Exponential Type

Orbital Integrals in Poly-Atoms 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""
