1. Record Nr. UNISALENTO991001275459707536

Autore	Etiemble, Renè
Titolo	Genese du mythe : 1869-1949 : bibliographie analytique et critique suivie d'un supplement aux iconographies / Etiemble
Pubbl/distr/stampa	[Paris] : Gallimard, [1968]
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Lingua di pubblicazione	Francese
Formato	Materiale a stampa
Livello bibliografico	Monografia

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Autore	Quinn Charles M
Titolo	Computational quantum chemistry [[electronic resource]] : an interactive guide to basis set theory / / Charles M. Quinn
Pubbl/distr/stampa	San Diego, Calif., : Academic Press, c2002
ISBN	1-281-05273-6 9786611052737 0-08-048853-6
Descrizione fisica	1 online resource (246 p.)
Disciplina	541.2/8/0285
Soggetti	Quantum chemistry - Data processing Gaussian basis sets (Quantum mechanics)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references (p. [229]-230) and index.
Nota di contenuto	Machine generated contents note: 1 Essential atomic orbital theory -- 11 Atomic orbitals for the hydrogen atom -- 12 Radial distribution functions for the hydrogen atom -- 13 Radial wave functions for many-

electron atoms -- 14 Slater-type orbitals -- 15 Gaussian-type functions-the Isto-3g) minimal basis set -- 16 isto-ng) basis sets -- 17 Scaling factors -- 18 The (4s/2s) basis set, polarization and scaling factors for molecular -- environments -- 19 Gaussian-lobe and other Gaussian basis sets -- 2 Numerical integration -- 21 Numerical integration -- 22 Application of Simpson's rule to calculate a normalization integral -- 23 Calculations of normalization constants over the angular coordinates -- 24 Numerical integration in a cylindrical volume: diatomic and linear -- molecular geometries -- 25 Calculation of the overlap integral between Is orbitals in a Gaussian -- basis -- 26 Designing Gaussian basis sets to model Slater orbitals -- 3 Orthonormality -- 31 Orthonormality in Slater orbital and basis set theory -- 32 Orthonormality and Slater orbitals -- 33 Orthonormality and Gaussian orbitals -- 34 Orthonormality and double-zeta Slater orbitals -- 35 Orthonormality and split-basis or double-zeta Gaussian basis sets -- 36 The Jacobi transformation, diagonalization of a symmetric matrix and -- canonical orthogonalization -- 37 The S-1/2 'trick' -- 38 Symmetric orthonormalization -- 4 The hydrogen atom - numerical solutions -- 41 Eigenvalue calculations for hydrogen based on analytical functions -- 42 Calculations using Slater orbitals -- 43 Calculations with Gaussian functions -- 44 Calculations with split-basis [split-valence] sets -- 45 Review of results for the ls and 2s orbital energies in hydrogen -- 5 The helium atom and the self-consistent field -- 51 Hartree's analysis of the helium atom problem -- 52 Calculations with modified hydrogen atom wave functions -- 53 The Hall-Roothaan equations, the orbital approximation and -- the modem Hartree-Fock self-consistent field method -- 54 Calculations using Slater DZ functions -- 55 Gaussian basis set calculations for the helium atom-two-electron -- integrals over Gaussian basis functions -- 56 A HFS-SCF calculation with split-basis 14-31) for helium -- 57 Helium, singlet and triplet excited states, electron spin and the role -- of the Exchange integral -- 6 One- and two-electron diatoms -- 61 Calculations using hydrogen Is orbitals -- 62 Sto-3g calculations for H2+ -- 63 Calculations using Gaussian basis sets with the exact evaluation of -- integrals using Fourier transforms -- 64 Calculations involving the two-electron terms; the Isto-3g) -- HF-SCF results for dihydrogen -- 65 The standard form for the results of HFS-SCF calculations -- 66 The Isto-3g) HFS-SCF calculation for HeH+ -- 67 Polarization functions, Gaussian lobes and higher-order Gaussian -- basis sets -- 68 Epilogue.

Sommario/riassunto

Computational Quantum Chemistry removes much of the mystery of modern computer programs for molecular orbital calculations by showing how to develop Excel spreadsheets to perform model calculations and investigate the properties of basis sets. Using the book together with the CD-ROM provides a unique interactive learning tool. In addition, because of the integration of theory with working examples on the CD-ROM, the reader can apply advanced features available in the spreadsheet to other applications in chemistry, physics, and a variety of disciplines that require the solution