Unified Treatment for Two-Center One-Electron Molecular Integrals Over Slater Type Orbitals with Integer and Noninteger Principal Quantum Numbers

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A unified expression has been obtained for two-center one-electron molecular integrals over Slater type orbitals with integer and noninteger principal quantum numbers by the use of the expansion formula for the product of two normalized associated Legendre functions. The presented expression for two-center one-electron molecular integrals contains the expansion coefficients $d_{us}^{kk'}$ and Mulliken integrals A_n and B_n. The efficiency of the presented calculation has been compared with that of other methods, indicating good convergence and great numerical stability for a wide range of quantum numbers, orbital exponents and internuclear distances.

Key words: Slater Type Orbitals; Noninteger Principal Quantum Numbers; Overlap Integrals; Nuclear Attraction Integrals.