On the Computation of Two-center Coulomb Integrals over Slater Type Orbitals Using the Poisson Equation

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In this paper, a new analytical formula has been derived for the two-center Coulomb integrals over Slater type orbitals using the Poisson equation. The obtained results from constructed computer program for the presented formula have been compared with the available literature and it is seen that the efficiency of the presented algorithm for a wide range of quantum numbers, orbital exponents and internuclear distances is satisfactory.

Key words: Coulomb Integral; Slater Type Orbital; Poisson Equation; Overlap Integral.