On the Evaluation Overlap Integrals with the Same and Different Screening Parameters Over Slater Type Orbitals via the Fourier-Transform Method

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Abstract: In this paper, derivation of analytical expressions for overlap integrals with the same and different screening parameters of Slater type orbitals (STOs) via the Fourier-transform method is presented. Consequently, it is relatively easy to express the Fourier integral representations of the overlap integrals with same and different screening parameters mentioned as finite sums of Gegenbauer, Gaunt, binomial coefficients, and STOs.

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