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On Evaluation of Overlap Integrals with Noninteger Principal Quantum Numbers

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Abstract: By use of complete orthonormal sets of ψ^{α} exponential-type orbitals (ψ^{α}-ETOs, α= 1,0, -1, -2, ...) the series expansion formulas for the noninteger n^{*} Slater-type orbitals (NISTOs) in terms of integer n Slater-type orbitals (ISTOs) are derived. These formulas enable us to express the overlap integrals with NISTOs through the overlap integrals over ISTOs with the same and different screening constants. By calculating concrete cases the convergence of the series for arbitrary values of noninteger principal quantum numbers and screening constants of NISTOs and internuclear distances is tested. The accuracy of the results is quite high for quantum numbers, screening constants and location of STOs.

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Key words: Slater-type orbitals, exponential-type orbitals, noninteger principal quantum numbers, overlap integrals

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