

On the Evaluation of Two-Center Overlap Integrals over Integer and Noninteger n -Slater-Type Orbitals

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Abstract: In this study, two-center overlap integrals over Slater-type orbitals (STOs) with integer and noninteger principal quantum numbers in unaligned coordinate systems have been calculated using formulas for overlap integrals in aligned coordinate systems obtained by the author's previous work (T. Özdoğan and M. Orbay, *Int. J. Quant. Chem.* 87 (2002) 15). The obtained results for integer case have been found to be in excellent agreement with the prior literature. On the other hand, to the best of authors knowledge, because of the scarcity of the literatures on the use of noninteger n -STOs in unaligned coordinate systems, the results for noninteger case have been tested with the limit of integer case, and good agreement has been obtained too.

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

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