On the Accurate Evaluation of Overlap Integrals over Slater Type Orbitals Using Analytical and Recurrence Relations

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In this study, using the analytical and recurrence relations suggested by the authors in previous works, the new efficient and reliable program procedure for the overlap integrals over Slater type orbitals is presented. The proposed procedure guarantees a highly accurate evaluation of the overlap integrals with arbitrary values of quantum numbers, screening constants and internuclear distances. It is demonstrated that the computational accuracy of the proposed procedure is not only dependent on the efficiency of formulas, as has been discussed previously, but also on a number of other factors including the used program language package and solvent properties. The numerical results obtained, using the algorithm described in the present work, are in complete agreement with those obtained using the alternative evaluation procedure. We notice that the program works without any restrictions and in all ranges of integral parameters.

Key words: Slater Type Orbitals; Overlap Integrals; Recurrence Relations; Auxiliary Functions.