Analytical treatment of two-center overlap integral with respect to same screening constants over Slater-type orbitals

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Abstract: By the use of Löwdin- α radial function, an alternative method is introduced for two-center overlap integral over Slater-type orbitals (STOs) at same screening constants (SSC). Notice that the overlap integrals with SSC have an important role in accurate evaluation of multicenter multielectron molecular integrals arising in combined Hartree-Fock-Roothaan (CHFR) theory. This approximation provides us simple and efficient expression for the two-center overlap integrals. To show the effectiveness of established formula we have compared our results with available literature data [1]. The method ensures high performance with a very short CPU time.

Keywords: Löwdin- α radial function, Hartree-Fock-Roothaan (CHFR) theory

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References

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