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Computation of Overlap, Kinetic and Nuclear Attraction Integrals by a Novel Method

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Abstract: A new way of computing overlap, kinetic and nuclear attraction integrals over Slater functions by means of optimized Gaussian expansion is proposed. This article is concerned with the construction of the general algorithm for evaluating the three integrals. These integral formulae presented in the form of a series whose terms are the analytical function of inter-atomic distances. In the present method, unlike many other popular methods, the numerical integration procedure is unnecessary since it does not contain the incomplete gamma function. The present scheme has been programmed in standard Fortran-77 and tested for various orbitals. The result of the calculation are compared with the literature data.

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