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Calculation of Multi-Center Integrals for the Region of Moderate and Weak Overlap

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Abdulhalik KARABULUT, Gökhan BUDAK, Lütfü DEMİR

Atatürk University, Sciences and Letters Faculty,

Department of Physics, 25240 Erzurum-TURKEY

Nagif Sefteroğlu NABIYEV

Bakü State University, Faculty of Physics, Bakü-AZERBAJCAN

Yusuf ŞAHİN

Atatürk University, Sciences and Letters Faculty,

Department of Physics, 25240 Erzurum-TURKEY

 [Keywords](#)
 [Authors](#)



chem@tubitak.gov.tr

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Abstract: In this study a general formula was established for multi-center integrals over Gaussian basis sets using the two-center expansion of nuclear attraction and electron repulsion potentials. The terms of the formula are the analytical functions of interatomic distances. Three kinds of integrals contained in these formulae can be evaluated analytically. In the presented method, unlike many other popular methods, the numerical integrations procedure is unnecessary since it does not contain the incomplete gamma function. A computer program was written and tested for various orbitals. The calculations show that the series converge very rapidly.

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