Full Papers

Evaluation of Two-center One- and Two-electron Integrals over Slater Type Orbitals

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摘要   A formulation previously presented by the authors for coulomb integrals was generalized to other two-center integrals, except exchange integral. Within this frame, molecular integrals were expressed in terms of some new functions closely related to the well-known incomplete gamma functions and these functions recursively evaluated. Special issues arising in the case of hybrid integrals were addressed, and the results were compared with the ones found in the literature.

关键词   overlap integral   hybrid integral   coulomb integral   Slater type orbital   elliptical coordinate

分类号

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