SYMMETRY RELATIONS BETWEEN TWO-ELECTRON INTEGRALS OVER H-SHELL ORBITALS OF FULLERENE C_{60}

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S u m m a r y

A method is elaborated that takes advantage of the linear relations, arised from the point symmetry of a molecule, between two-electron integrals defined on symmetry molecular orbitals. Using the symmetry similarity principle within the model with two-center electron-electron interaction, a simple technique is developed enabling to represent each integral from the complete set as an expansion of a few independent integrals. The technique is applied to the set of integrals originating from the H-shell of fullerene C_{60}, which is important for the calculations of C_{60} multicharged cations. For the five-fold irreducible representation, the C_{60} basis symmetry orbitals and integral expansions are obtained in a form convenient for calculations. The reduced set involves only five independent integrals instead of 120 ones in the general case. The obtained expansions are valid for ab initio calculations involving three- and four-center atomic integrals.