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Explicit Formulae for the Calculation of Molecular Multipole Moments Integrals Over Slater Type Orbitals.
 Graovac, A.; Maksić, Z.B.; Mikac, J. (Rudjer Bošković Inst., Zagreb, Yug.) CCACAA 1977, 49(1) SYUD 77/001, 46 pp.
 (Engl.)

A method for the rigorous calculation of the molecular multipole moments integrals over Slater type atomic orbitals is presented. It is shown that the multipole moments integrals are easily reduced to linear combinations of two-centre overlap integrals which can be routinely calculated.

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Descriptors	1 dipole moments	3 molecular multipoles	5 Slater type orbitals	7
	2 molecular integrals	4 quadrupole moments	6	8

Synopsis/informative abstract	A47	Abstr. numbers	CCACAA-SYUD 77/001
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Multipole moments of the electronic charge distribution in molecules play an important role in the description of physical and chemical properties of molecules and their interactions. For example, dipole moment μ provides information about electronic distribution at medium distances from a suitable origin of a coordinate system and second moments $\langle x^2 \rangle$, $\langle y^2 \rangle$ and $\langle z^2 \rangle$ describe the outer shape of the electronic charge cloud. The latter entities are also closely related to the diagonal components of the diamagnetic susceptibility tensor. Third and higher moments are connected with second and third-order nonlinear optical effects which are conveniently studied by laser light sources. The electrostatic interaction between molecules is easily expressed in terms of multipole moments and this type of approach seems to be very useful for investigation of large molecules of biological importance as well as for a study of certain types of chemical reactions. Finally, dipole, quadrupole and octupole moments are highly sensitive to the quality of the molecular wave functions and serve as very good probes for a quantitative appraisal of semiempirical charge distributions in molecules. In this note we report on a method for the exact calculation of the multipole moments integrals over Slater type atomic orbitals (STO). The multipole moments of the form $x^i y^j z^k$ up to the third order ($1 \leq i + j + k \leq 3$) were considered. Their matrix elements are reduced to linear combinations of two-centre overlap integrals which are routinely calculated in numerous programmes now in use in quantum chemistry. Master formulas for the calculation of multipole moments integrals STOs up to the fifth period for first moments, fourth period for second moments and third period of the Mendeleev system of elements for third moments are given. Full paper involves details of the numerical procedure, worked examples and master formulas.

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