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Electric multipole moments of some diatomic molecules Molecules

M. Özgür SEZER, Ayhan ÖZMEN, and Hüseyin YÜKSEL
Department of Physics, Selçuk University, Faculty of Science and Literature, Konya-TURKEY
e-mail: msezer@selcuk.edu.tr

Abstract: Molecular Electric Multipole Moment (MEMM) integrals have been derived for diatomic molecular systems, and then some lower multipole moments as dipole moments and quadrupole moments have been calculated for some diatomic molecules. The calculations have been performed by using our analytical formula over Slater-Type orbitals (STOs) with Cade and Huo's basis sets and the GAMESS program package working with Gaussian-Type basis sets (GTOs). The expressions which involve factorials are given in terms of binomial coefficients in order to speed up calculations. The results have been obtained in agreement with data found in the literature.

Key Words: Multipole moments, quadrupole moments, dipole moments, Slater-type orbitals