

# Quadrupole moments, dipole quadrupole A and quadrupole C polarizabilities by means of perturbation theory

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Quadrupole moments, dipole quadrupole polarizability A, and quadrupole polarizability C values have been obtained for a set of organic molecules, in both the ground and first singlet excited states, by means of Rayleigh-Schrödinger perturbation theory. Computations for  $\pi$  systems have been carried out using the PPP-SCF procedure. Results are discussed through the paper and compared with available experimental and theoretical information. Quadrupole moments are shown to be very sensitive to the quality of the wave functions, and the A and C polarizabilities are highly dependent on geometries. Copyright © 1979 John Wiley & Sons, Inc.