

Singlet and triplet excited state electric dipole polarizabilities of conjugated hydrocarbons

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First excited singlet and triplet electric dipole polarizabilities are reported. The π polarizability is calculated by means of a modified Rayleigh-Schrödinger perturbation theory and an SCF-LCAO basis. The σ contribution is included by an additive scheme. The polarization of the π electrons is partially accounted for through an empirical correction. Results compare satisfactorily with a configuration interaction perturbation calculation. Copyright © 1976 John Wiley & Sons, Inc.