Comparison of several expansions in the calculation of static electric dipole ? polarizability of conjugated molecules by pertubation theory. The ground and the first excited singlet states

Matzke, P.

Chacon, O.

Sanhueza, E.

Trsic, M.

Ground and excited singlet state dipole electric ? polarizabilities of a set of conjugated molecules are calculated. Second order perturbation theory is used in the Epstein?Nesbet and Möller?Plesset versions. Hückel and SCF?LCAO?MO are used alternatively as a basis. The Möller?Plesset?SCF?LCAO?MO calculation appears well related to experimental values. Copyright © 1972 John Wiley & Sons, Inc.