

hyperpolarizability (of n th order)

The energy of a molecule in an external electrostatic field can be expanded as

$$E = E^0 - \mu_i F_i - \frac{1}{2} \alpha_{ij} F_i F_j - \frac{1}{6} \beta_{ijk} F_i F_j F_k - \frac{1}{24} \gamma_{ijkl} F_i F_j F_k F_l - \dots$$

where E^0 is the unperturbed energy, F_i is the component of the field in the i direction, μ_i is the permanent dipole moment, α_{ij} is the polarizability tensor, and β_{ijk} and γ_{ijkl} are the first and second hyperpolarizability tensors, respectively. β is a third order symmetric tensor that measures the second order response of the molecular electric dipole moment to the action of an external electric field and is thus often referred to as dipole hyperpolarizability.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1946