

Theory of molecular orbital energy shifting induced by electrostatic external effects

Contreras, Renato R.

Aizman, Arie J.

The Self Consistent Reaction Field (SCRF) theory of electrostatic medium effects representation is used as the basis to derive the molecular orbital energy shifting induced by electrostatic external effects, coming from the interaction with a highly polarizable medium. A Perturbation?Variation methodology is used to perform the theoretical analysis. Under a first order perturbation approach, the shifting induced on the molecular electronic levels appears to be mainly dependent on the electronic polarization of the particular molecular orbital involved. As a result, it appears that the molecular orbital energy levels do not shift in a trivial constant amount by solvation, as it has been currently assumed. The result of our theoretical analysis shows that the solute electronic polarization term may be a relevant contribution to the molecular orbital energy changes induced by the environment. As an illustration of the usefulness of the present analysis, the alpha effect towards nucleophil