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Coulomb repulsion

The potential energy component corresponding to the electrostatic interaction between each pair of charged particles:

$$V = \frac{1}{4\,\pi\,\varepsilon_0} \sum_i \sum_{j<i} e_i\, e_j\, \Delta r_{ij}$$

where ε_0 is the permittivity of a vacuum, Δr_{ij} is the distance between the two particles, and e_i and e_j are the charges on particles i and j. In molecular orbital theory, the electrostatic repulsion between the two electrons occupying the orbitals Ψ_i and Ψ_j. In the Hartree–Fock method, the mean Coulomb repulsion is determined by the value of the Coulomb integral

$$J_{ij} = \int\int \Psi_{i*}(\mathbf{r}_1)\, \Psi_i(\mathbf{r}_1) \left(\frac{e^2}{r_{12}}\right) \Psi_{j*}(\mathbf{r}_2)\, \Psi_j(\mathbf{r}_2) \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 = \, < ij \mid ij >$$

See also: exchange repulsion

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1932

