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exchange repulsion

Also contains definition of: exchange integral

The correction to the Coulomb repulsion between two electrons in orbitals Ψ_i and Ψ_j for the case when the electrons possess parallel spins. It is to be subtracted from the Coulomb repulsion to give the total energy of the electron–electron interaction. In the Hartree–Fock theory the magnitude of the exchange repulsion is given by the exchange integral

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

For the case of electrons with opposite spins K_{ij} vanishes.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

