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Summary of scientific research

A general method to explain the orientation and stereoselection in chemical reactions is given based on the model in which the electron delocalization between the highest occupied molecular orbitals of a reactant and the lowest unoccupied molecular orbitals of a reagent plays an essential role. These particular orbitals are popularly called "frontier orbitals". The symmetry of frontier orbitals is shown to be significant in various sorts of cyclic additions and intramolecular rearrangements.

A mathematical formulation of reaction coordinate, named as "intrinsic reaction coordinate", is carried out with respect to the path of each elementary reaction. This approach enables calculation of the change of energy and geometry of reacting molecules and various correlation diagrams along the reaction path, as well as calculation of wave-mechanical absolute rates of chemical reactions. The same approach elucidates the mathematical nature of chemical reaction paths in the potential energy hyperspace, showing that the path of a chemical reaction is controlled by various variational formulae. The correlation diagram concerning the vibrational modes and frequencies along the reaction path is shown useful in connection with laser-induced

mode-selective reactions and chemical lasers.

The diagonalization of delocalization energy gives a quantitative representation of the frontier orbitals "for the reaction species", which is combined with the intrinsic reaction coordinate approach giving a means of "visualization" of a chemical reaction.
