The reaction simplex,

a concept for modeling

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Pseudounimolecular rearrangement reactions are represented as being characterized by an initial, reactant, conformation R, an intermediate, transitional, one called T, and a final, product, conformation P. A suitable multidimensional quotient space, where translations and irrelevant rotations are removed, serves to define the triangle RTP as the reaction simplex. The process is reduced to a two dimensional quantum mechanical problem. London's four orbital model for the AB + CD → AC + BD rearrangement is adapted to define two electronic energy surfaces from the knowledge of ground state energies and Hessians at the three vertices of the simplex.

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