## potential-energy profile

A curve describing the variation of the potential energy of the system of atoms that make up the reactants and products of a reaction as a function of one geometric coordinate, and corresponding to the 'energetically easiest passage' from reactants to products (i.e. along the line produced by joining the paths of steepest descent from the transition state to the reactants and to the products). For an elementary reaction the relevant geometric coordinate is the reaction coordinate; for a stepwise reaction it is the succession of reaction coordinates for the successive individual reaction steps. (The reaction coordinate is sometimes approximated by a quasi-chemical index of reaction progress, such as 'degree of atom transfer' or bond order of some specified bond.)

See also: potential-energy (reaction) surface, Gibbs energy diagram

## Source:

PAC, 1994, 66, 1077 (Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)) on page 1151

PAC, 1996, 68, 149 (A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)) on page 176