

### **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*.  
1994, 66, 1151; 1996, 68, 176