

Gibbs energy of activation (standard free energy of activation), $\Delta^\ddagger G^\circ$

The standard Gibbs energy difference between the transition state of a reaction (either an elementary reaction or a stepwise reaction) and the ground state of the reactants. It is calculated from the experimental rate constant k via the conventional form of the absolute rate equation:

$$\Delta^\ddagger G = R T \left[\ln\left(\frac{k_{\text{B}}}{h}\right) - \ln\left(\frac{k}{T}\right) \right]$$

where k_{B} is the Boltzmann constant and h the Planck constant ($\frac{k_{\text{B}}}{h} = 2.083\,58 \times 10^{10} \text{ K}^{-1} \text{ s}^{-1}$). The values of the rate constants, and hence Gibbs energies of activation, depend upon the choice of concentration units (or of the thermodynamic standard state).

See also: enthalpy of activation, entropy of activation

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1118

PAC, 1996, 68, 149 (*A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)*) on page 166