Theoretical aspects of the activation and its access to the activation energies of gas phase chemical reactions

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Abstract

Various bonds in molecules accumulate energies under rising temperature until the energies are sufficient to promote dissociation. The activation energy of a chemical reaction AB → A + B and the bond dissociation energy, D(A-B) are calculated on the basis of the A—B bond stretching vibration (cm-1). The activation energies, Ea = 883, 407, 249.31, and 437.7 kJmol-1 are calculated for nitrogen, hydrogen chloromethane and water respectively. The dissociation energies D(N-N) = 945.07, D(H-H) = 435.5, while for C2H5Cl the D(C-H) = 409.22 and D(C-Cl) = 341.75 kJmol-1 are also calculated. In each case, the theory confirms the experimental findings