

bond-dissociation energy (BDE)

in theoretical chemistry

For a diatomic molecule, the maximum vibrational energy that a molecule can have prior to its decomposition into the ground electronic states of the constituent atoms (spectroscopic bond-dissociation energy, D_e). The D_e value is related to the chemical dissociation energy: $D_0 = D_e - E_{\text{vib}}(0)$, where $E_{\text{vib}}(0)$ is zero-point vibrational energy. This definition is usually extended to the dissociation of polyatomic molecules into certain molecular fragments through homolytic or heterolytic bond cleavages.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1928