

Morse potential

The empirical function relating the potential energy of a molecule to the inter-atomic distance r accounting for the anharmonicity (see harmonic approximation) of bond stretching:

$$E(r) = D_e \{ 1 - \exp[-a(r - r_e)] \}^2$$

where D_e is the bond-dissociation energy, r_e is the equilibrium bond length, and a is a parameter characteristic of a given molecule.

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