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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:

$$E(r) = D_e \left(1 - e^{-a\,(r - r_e)}\right)^2$$

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.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1953

