

Energy Formula and Potential Distribution of Diatomic Molecules

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David von Seggern
(vonneg@seismo.unr.edu) University of Nevada
July 2012, page 10
DIGITAL OBJECT IDENTIFIER
<http://dx.doi.org/10.1063/PT.3.1619>
The article by Thorne Lay and Hiroo Kanamori is an interesting one. It discusses the energy released by the 1995 Great Hanshin earthquake. The authors estimate that the earthquake released about 100 megajoules of energy. This is a very large amount of energy, but it is only a fraction of the energy released by a 100-megaton explosion. The authors also discuss the energy released by the 1964 Chikyu earthquake. They estimate that this earthquake released about 100 megajoules of energy. This is also a very large amount of energy, but it is only a fraction of the energy released by a 100-megaton explosion. The authors conclude that the energy released by earthquakes is much smaller than the energy released by nuclear weapons.

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By the act of hitting a ball with a bat, one calculates the force energy to deliver the ball to its new location, but one must also take into account that the ball extended its energy release to that which became struck by the ball as its momentum ceased and passed energy to the struck item. Therefore the parameters of the damage extend into the future when the received energy to that pushed upon later becomes released in a new event. Perhaps calculations of one added that in while another's calculations did not. E.M.C.
Written by Edgar McCarvill, 14 July 2012 19:59

Energy Formula and Potential Distribution of Diatomic Molecules*

Taking as general expression of a diatomic molecular potential $V(r)$ the following one,

$$\left. \begin{aligned} V &= -D + D\xi^2, \quad 1 - \xi = \frac{(1+a)(1+c)}{1+b} \frac{x+b}{(x+a)(x+c)}, \\ x &= e^{(1+k)\rho}, \quad \frac{1}{1+k} = \frac{1}{1+a} + \frac{1}{1+c} - \frac{1}{1+b}, \\ \rho &= [\hbar\nu_e/2(B_e D)^{\frac{1}{2}}](r-r_e)/r_e, \end{aligned} \right\} \quad (1)$$

r_e being the equilibrium distance of the atoms and D , B_e and $\hbar\nu_e$ well-known spectroscopic constants, the energy formula may be expressed as follows,

$$\left. \begin{aligned} 1 - \left(-\frac{E}{D}\right)^{\frac{1}{2}} &= \frac{\hbar\nu_e}{2D} \left(n + \frac{1}{2}\right) + \frac{A(\hbar\nu_e/2D)^2(n + \frac{1}{2})^2}{1 - \chi(\hbar\nu_e/2D)(n + \frac{1}{2})}, \\ A &= \frac{1}{2}(1 - a_2), \quad \chi = 1 - a_2 + \frac{a_2 - a_4}{1 - a_2}, \end{aligned} \right\} \quad (2)$$

$$\left. \begin{aligned} \rho &= \frac{1}{1+k} \log \frac{1}{1-\xi} \left\{ 1 + k\xi - \frac{2k_1 k_2 (1+k)\xi^2}{1 + (k_1 + k_2 + 2k_1 k_2)\xi + \sqrt{[1 + (k_1 + k_2 + 2k_1 k_2)\xi]^2 - 4k_1 k_2(1+k_1)(1+k_2)\xi^2}} \right\}, \\ k_1 &= \left(\frac{1}{1+b} - \frac{1}{1+a}\right)(1+k), \quad k_2 = \left(\frac{1}{1+b} - \frac{1}{1+c}\right)(1+k). \end{aligned} \right\} \quad (5)$$

If now this energy formula can be adjusted to the observed vibrational energy levels of a molecule, the coefficients a_2 and a_4 are already given. The coefficient a_1 may easily be found from the first order dependance of B upon the quantum number n . Thus the constants of the potential curve, k , k_1 and k_2 , or, a , b and c are defined and may be calculated from a_1 , a_2 and a_4 and so we have an analytical expression of the potential distribution of the molecule.

In Fig. 1 some potential curves are given, the solid curve being the well-known potential curve given by Morse.¹ With the same curvature and the same asymmetry at the minimum point the dotted curves are narrower in

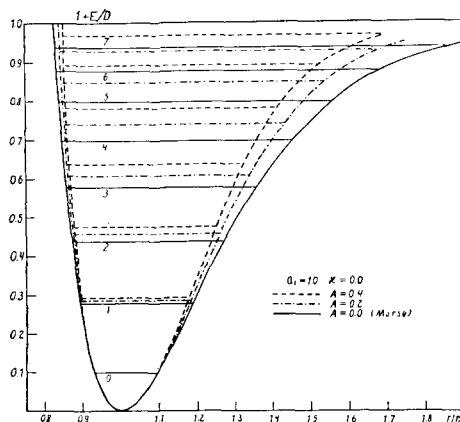


FIG. 1. Dependence of the upper levels of the narrowness of the potential curves.

a_2 and a_4 being coefficients in the expansion of $d\rho/d\xi$ in power series of ξ ,

$$d\rho/d\xi = 1 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + \dots \quad (3)$$

The rotational constant B depends upon the vibrational quantum number n in the following way,

$$\left. \begin{aligned} B &= B_e - \alpha(n + \frac{1}{2}) - \alpha_2(n + \frac{1}{2})^2 - \dots \\ \alpha/B_e &= \frac{\hbar\nu_e}{2D} \left[3a_1 \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right) - 3 \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right)^2 \right], \\ \alpha_2/B_e &= \left(\frac{\hbar\nu_e}{2D} \right)^2 \left[\left(\frac{15}{4} a_2 - 2a_1 a_2 \right) \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right) \right. \\ &\quad \left. - \left(3a_2 + \frac{45}{8} a_1^2 \right) \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right)^2 + 15a_1 \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right)^3 \right. \\ &\quad \left. - \frac{15}{2} \left(\frac{2(B_e D)^{\frac{1}{2}}}{\hbar\nu_e} \right)^4 \right]. \end{aligned} \right\} \quad (4)$$

The coefficients a_1 , a_2 , a_3 , a_4 , may be derived from the expression

the upper part, thus raising progressively the upper energy levels.

In Fig. 2 quite another variation possibility of the curves is illustrated, the energy formula being unaltered and only the symmetry of the curves being changed.

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¹ P. M. Morse, Phys. Rev. **34**, 57 (1929).

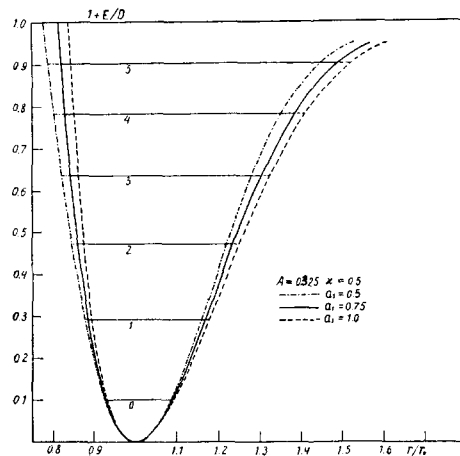


FIG. 2. Potential curves with different asymmetry but with identical energy levels.