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# BOOK OF ABSTRACTS

# Application of the Morse Approximation for the Study of Noncovalent Interactions

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Despite a very rough approximation, the Morse model potential $M(r)$[1] is widely used in different fields of physical chemistry including the studies of intermolecular interactions (hydrogen bonding, properties of crystals, adsorption, etc.). The features of its practical use are presented based on articles;[2-4] the distortions are described which are determined by the approximation of the original electronic term $U(r)$; the anharmonicity function is introduced, which is important for optimization of the problem statement; several examples of recent papers highlighting the effectiveness of the approach are given.

The difference $\delta(r) \equiv U(r) - M(r)$ as a function of the vibrational quantum number v is used to evaluate the distortions. Based on the literature data, two types of the Morse potential were calculated for a number of diatomic molecules according the article[1] for two sets of initial parameters: $r_e$, $\omega_e$, $\omega_e x_e$ ($M1$) and $r_e$, $\omega_e$, $D_e$ ($M2$). The empirical function of anharmonicity $\omega x(v)$ is introduced as a progression of energy differences of adjacent vibrational levels. This function characterizes the anharmonicity at the certain region of the potential well $U(r)$ near the level $v$ and shows the deviation of Morse models $M1$ and $M2$ from initial term $U(r)$. The form of the functions $\delta(r)$ and $\omega x(v)$ for several molecules are presented and some generalizations are made.

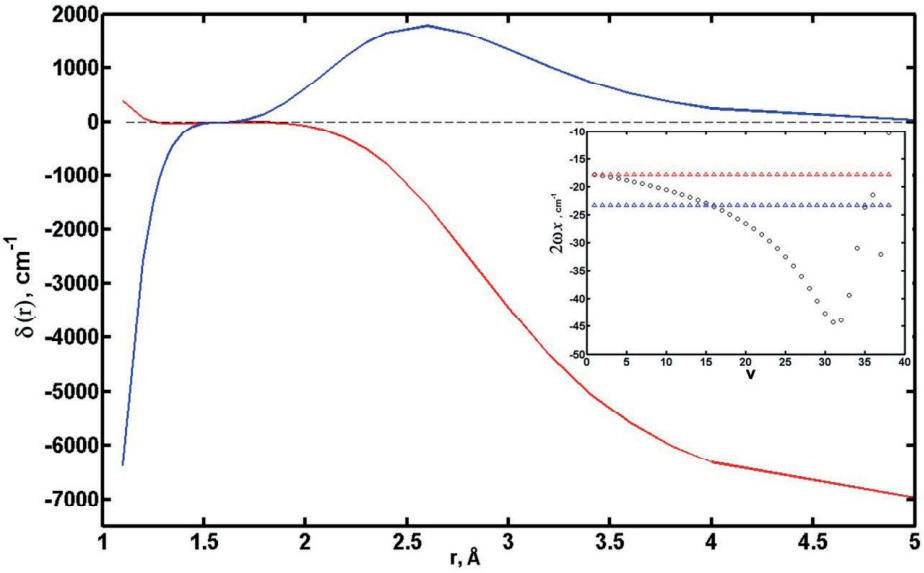


**Figure 1.** Deviations of Morse models $M1$ (red) and $M2$ (blue) from initial term $X^1\Sigma_g^+$ for $B_2$ molecule. Inset – anharmonicities for $U(r)$ (black), $M1$ (red) and $M2$ (blue)

**References**

1. P. M. Morse, Phys. Rev. **1929**, 34, 57.
2. G. S. Denisov, I. G. Denisov, Spectr. Acta A **2021**, 262, 120111.
3. G. S. Denisov, K.G. Tokhadze, Opt. Spectrosc. **2021**, 129, 1375.
4. G. S. Denisov, Opt. Spectrosc. **2022**, 130, 1306.