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# Predicting anharmonicity constants using machine learning

Considering anharmonic effects is essential to accurately describe vibrational, spectroscopic and thermodynamic properties of molecular systems. Recently, it has been shown that introducing anharmonic formalism into the quantum cluster equilibrium (QCE) program improves the results of the calculations [1]. It is possible to calculate anharmonic frequencies [2]. However, such calculations are tedious and computationally expensive, therefore it is of prime interest to apply machine learning techniques to overcome this task. In this work we study a variety of molecular clusters of different sizes consisting of HX, CH3X, C2H5X (X = F, Cl, Br) monomers. Our dataset features consist of normal mode coordinates as well as harmonic frequencies, anharmonic frequencies and intensities of the fundamental and first overtone modes. Symmetry and structural descriptors such as internal coordinates are also taken into account. Anharmonicity constants are extracted from the vibrational energy levels of the Morse oscillator. Later on, various machine learning algorithms are applied for the classification and regression purposes. Our results show that while stretching vibration modes have positive anharmonicity constants, the low frequency bending and torsional modes often exhibit negative values. With this we were able to classify the anharmonicity constants according to the type of vibration such as stretching, bending, or internal rotations and translations. Regression algorithms were able to provide an estimate of the anharmonic frequencies.

References:
[1] J. Chem. Phys. 146, 124114 (2017)
[2] J. Chem. Phys. 105, 10332 (1996)

**Primary author:** KHANIFAEV, Jamoliddin (PhD student)

**Co-author:** VON DOMAROS, Eva

**Presenter:** KHANIFAEV, Jamoliddin (PhD student)

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