Prediction of NH stretching frequencies of intramolecularly hydrogen-bonded primary amines

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Rok wydania

2026

Czasopismo

Chemical Physics

Numer woluminu

607

Strony

113213/1-113213/9

DOI

10.1016/j.chemphys.2026.113213

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The NH stretching frequencies of a series of intramolecularly hydrogen-bonded (HB) amines are investigated based on Car-Parrinello Molecular Dynamics (CP-MD) as well as by static Density Functional Theory (DFT) approach. CP-MD simulations are employed to investigate the time-evolution of interatomic distances in the hydrogen bond and to derived spectroscopic parameters in a set of primary enaminones. The vibrational features are investigated based on the Fourier transform of the autocorrelation function of atomic velocity. Harmonic NH stretching frequencies computed with DFT at the B3LYP/6-311++G(d,p) level of theory show a good correlation with experimental results, whereas this is not the case using the anharmonic Generalized 2nd-order Vibrational Perturbation Theory (GVPT2) approximation. The QTAIM approach predicted the hydrogen bonding strength to be within the −6.21 to −13.40 kcal/mol range, and the quantitative predictions of QTAIM were in agreement with semi-quantitative estimates based on CP-MD and harmonic DFT calculations.

Słowa kluczowe

Intramolecular hydrogen bond, Car-Parrinello molecular dynamics, DFT, Harmonic frequencies, Anharmonicity, QTAIM

Adres publiczny

http://dx.doi.org/10.1016/j.chemphys.2026.113213

Strona internetowa wydawcy

http://www.elsevier.com