

IR and Raman spectra of N₂H₂

See the experimental spectrum at: www.webbook.nist.gov

Consider the cis, trans and iso conformers; use the correct symmetry for each conformer

B3LYP/6-31G(d) Use MP2/cc-pVDZ for SP on optimized conformers

Calculate IR and Raman spectra; express the normal modes using the internal coordinates; use scaling factors from: <http://cccbdb.nist.gov/>

Freq(Intmodes)

Calculate IR and Raman spectra for the deuterium-substituted molecule

Freq(Readiso)

0 1

molecule specification

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300.0 1.0 (temperature and pressure)

14

14

2

2

Calculate the anharmonic vibrational spectrum

Freq(anharm)