Assigning Vibrational Modes of Ethanethiol with Computation and Matrix Isolation Infrared Spectroscopy

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The Vasiliou Lab used computation (Gaussian 09) along with Matrix isolation infrared spectroscopy to study the vibrational structure of the ethanethiol (CH_3CH_2SH). Methods (including RHF, MP2, B3LYP, O3LYP, M06 and wB97X-D) and the basis set aug-cc-pV(T+d)Z were used to compute the harmonic vibrational frequencies of the gauche and trans conformers of ethanethiol. Comparing the calculated IR frequencies with experimental MIIR spectra of ethanethiol led to peak assignments for 18 gauche and 16 trans vibrational modes. Correcting for anharmonicity resulted in more predictive IR vibrational frequencies of ethanethiol.