Two-dimensional surface scan and analysis of vibrational spectra of 3,3-difluoropropanal based on ab initio and normal coordinate calculations

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Abstract: The conformational behavior and structure of 3,3-difluoropropanal were investigated by utilizing ab initio calculations with 6-31G** basis set at RHF, MP2, and B3LYP levels. The molecule was predicted to exist in ii complex mixture of conformers at ambient temperatures. Two-dimensional single point surface scan for the rotations of both the CHO and CHF2 rotors was calculated at RHF and MP2 levels. Full optimization was then performed at the possible minima and at the transition states. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calculations for the three most stable cis-gauche, gauche-cis and gauche-gauche conformers of the molecule. Vibrational Raman and infrared spectra of the mixture of the stable conformers were computed at 300 K.