Infrared and Raman spectra, vibrational assignments and potential energy distributions for 3-butyral by ab initio and normal coordinate calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The vibrational frequencies were computed at HF/6-311G* level for the cis (acetylenic group is cis with respect to carbonyl group) and gauche conformers of 3-butyral. Normal coordinate calcns. were carried out and potential energy distributions among symmetry coordinates were calcd. for the two stable conformers of the mol. The computed vibrational frequencies were scaled and compared to those obsd. exptl. for similar mols.