

Infrared and Raman spectra, vibrational assignments and potential energy distributions for 3-butyne 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-butyne. Normal coordinate calculations were carried out and potential energy distributions among symmetry coordinates were calculated for the two stable conformers of the molecule. The computed vibrational frequencies were scaled and compared to those observed experimentally for similar molecules.