

Theoretical calculations of vibrational frequencies and derived potential energy distributions from normal coordinate analyses for 2,3-butadienal. Forner, Wolfgang; Badawi, Hassan M

Abstract

The vibrational frequencies were computed at HF/6-31G** level for the cis and trans conformers of 2,3-butadienal. 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.