

**Density functional calculations of C-P rotational barrier and vibrational wavenumbers for vinyl phosphonic dichloride and difluoride.** Badawi, H. M.; Forner, W

**Abstract**

The structure and conformational stability of vinyl phosphonic dichloride and difluoride were studied using ab initio calcns. at DFT-B3LYP/6-311++G\*\* level. From the calcns. the mols. were predicted to exist in cis.dblarw.gauche conformational equil. with the cis (phosphonic O eclipses the vinyl group) being the predominant conformer at ambient temp. The asym. potential function for the internal rotation was detd. for each of the two mols. The vibrational frequencies were computed. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the two mols. in the cis and the gauche conformations.