

Density functional calculations of C-P rotational barrier and vibrational wavenumbers for vinyl phosphonic dichloride and difluoride

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Abstract: The structure and conformational stability of vinyl phosphonic dichloride and difluoride were investigated using ab initio calculations at DFT-B3LYP/6-311 + +G** level. From the calculations the molecules were predicted to exist in cis \leftrightarrow gauche conformational equilibrium with the cis (phosphonic oxygen eclipses the vinyl group) being the predominant conformer at ambient temperature. The asymmetric potential function for the internal rotation was determined for each of the two molecules. The vibrational frequencies were computed. Normal coordinate calculations were carried out and potential energy distributions were calculated for the two molecules in the cis and the gauche conformations.