Theoretical C-As rotational barrier, vibrational wavenumbers, and potential energy distributions for vinyl arsonic dichloride and difluoride

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Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 546 **Pages:** 231-241

Abstract: The structure and conformational. stability of vinyl arsonic dichloride CH2=CHAsCl2O and difluoride CH2=CHAsF2O Were investigated using ab initio calculations at DFT-B3LYP/6-311++G** level. From the calculations the molecules were predicted to exist in cis double left right arrow gauche conformational equilibrium with the cis (arsonic 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 (PED) were calculated for the two molecules in the cis and the gauche conformations.