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ACCEPTOR PROPERTIES AND CONFORMATION ISOMERISM IN CH_2=CH–PX_2 (X = F OR Cl) COMPOUNDS

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ABSTRACT

Ab initio calculations of CH_2=CH–PF_2 and CH_2=CH–PCl_2 were performed to investigate their conformational isomerism. It has been shown that both compounds have two conformers: the *cis* and the eclipsed. The concept of group orbital interactions was used to analyse the electronic structure and geometry of these molecules. The most stable conformer of CH_2=CH–PX_2 has a *cis* orientation of the phosphorus lone pair and the CH_2=CH group due to the alkene–PX_2 hyperconjugation. From PMO and Mulliken population analysis, the PX_2 fragment acts as a π acceptor.

INTRODUCTION

Many molecular properties can be rationalized on the basis of the symmetry properties of molecular wavefunctions, e.g. classification the molecular states, calculation of the transition probabilities and detection of selection rules for electronic transitions [1,2] as well as the examination of the stereochemistry of polycyclic reactions. To predict the structure of organic compounds, it can be helpful to examine the π–π' interactions, which in many cases determine the relative stability of the conformers [3,4]. Therefore, a quantum-chemical study of the structure of unsaturated compounds allows dominating interactions to be characterized and allows discussion of some of their physical and chemical properties. In this paper we discuss the conformational studies made on derivatives of CH_2=CH–PX_2 (X = F or Cl).

RESULTS AND DISCUSSION

Conformational isomerism of CH_2=CH–PX_2 compounds

Recently a lot of experimental evidence concerning the geometry and electronic structure of derivatives of monoarylphosphines $ArPX_2$ and vinylphosphines has been obtained [5–8]. These phosphorus compounds have quite dif-

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