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A Computational Study to Find the Vibrational Modes Connected with Specific Molecular Structures of Calculated Compound

Golrokh Mahmoudzadeh[*]

Department of Chemistry, Arak Branch, Islamic Azad University, Arak, Iran

*Corresponding author *E-mail:* *gmahmoudzadeh@yahoo.com*

ABSTRACT

The purpose of this research is to provide a deeper understanding of the planar high- symmetry configuration instability. In the ideal case, the distortion corresponds to the movements of nuclei along normal modes that belong to non-totally symmetric irreps of the high symmertry (HS) point group of molecule. The analysis of the structural distortion from the HS nuclear arrangements of the JT active molecules presents a challenge because of the superposition of the effects produced by many different normal modes. It is shown that the instability of planar configurations of Tetrafluoroethylene radical anion, $CF_2 = CF_2^-$ molecule, leading to symmetry breaking and distortions is induced by the pseudo Jahn-Teller effect (PJTE). It was proved that the PJTE is the only source of instability of high-symmetry configurations of molecules. Therefore, the instability of planar configuration leading to symmetry breaking and distortions is induced by the pseudo Jahn-Teller effect (PJTE). In other words, in the studied molecule, descent in symmetry is associated with increasing the stability of molecule, i.e. the more curvature of the lower of curve have played a major role in stabilization energy so that the increasing of stability is attributed to the pseudo Jahn-Teller effect stablization energy (PJTE stabilization energy).

Keywords: Symmetry Breaking, Imaginary Frequencies and Trans-bent configuration, pseudo Jahn-Teller effect (PJTE).

Introduction

Quantum mechanical description of the changes in electronic structure due to distortions in molecular shape and vice versa is given in the form of the vibronic coupling theory. Probably, the most famous concept based on this theory is the Jahn−Teller (JT) effect. The JT theorem states that a molecule with a degenerate electronic state spontaneously distorts along a non-totally symmetric vibrational coordinates. This removes the degeneracy and lowers the energy. In fact, the vibronic coupling, correlation between electronic states and vibrational motion of nuclei, describes all spontaneous symmetry breaking distortions, attributed to the JT, Renner-Teller and pseudo JT effects [1-5]. Tetrafluoroethylene radical anion, CF2 = CF2− is an important basic constituent of the family of perfluoroalkene radical anions and serves as a prototype of such anions. In this paper, three distortion modes, Trans (b2g) and cis (b3u) bending and twisting (au), of tetrafluoroethylene radical anion are discussed as the vibrational modes connected with specific molecular structures of calculated compound. The change configuration from planar to Trans - bent geometry by Trans –bent modes of a CF2=CF2- molecule are defined as a lowering of symmetry from planar D2h to C2h symmetry. Therefore in this research, our study carried out on the tetrafoluroethylene anion via TD –DFT and CI-singles (CIS). Time-dependent density functional theory (TD-DFT), which is one of the most popular tools in the study of excited states of molecular systems, was used to study the electronic configuration of the planar and vibrational modes connected with specific molecular structures of compound [6].

Computational Details

In this study, geometric optimizations and frequency calculations are carried out for singlet state of Tetrafluoroethylene radical anion [C2F4] - in planar structuers. All calculations were performed with the Gaussion 09 [7] suite. Hartree-Fock calculations for the structural