ELECTRONIC CONTROL OF MOLECULAR CONFIGURATION INSTABILITY VIA VIBRONIC COUPLING. PSEUDO JAHN-TELLER STABILIZATION OF VERTICALLY EXCITED STATES OF F_2CO, N_2H_2 AND H_2C_2O MOLECULES

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Abstract. The pseudo Jahn-Teller effect is employed to explain the origin of distortions of carbonyl fluoride, diazene and ketene molecules in the lowest singlet and triplet excited states. The ground state and the excited electronic states of considered molecules were calculated by *ab initio* SCF CI method with the use of the 631G-type basis set. The corresponding pseudo Jahn-Teller coupling constants are estimated by fitting the *ab initio* data for the adiabatic potential curves of the molecules to the general formula, obtained from the vibronic theory. With these data an explanation of both the larger instability of the triplet excited states as compared with the singlet ones and the elongation of the corresponding bond distances in the excited states is obtained.

Keywords: Pseudo Jahn-Teller effect, stereochemistry, excited states, carbonyl fluoride, diazene, ketene.