

Abstract Submitted
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Theoretical Electronic Structure of Fluoromethanes and dissociation pathways¹ JUAN C. POVEDA, ALFONSO GUERRERO, IGNACIO ÁLVAREZ, CARMEN CISNEROS, Laboratorio de Colisiones Atómicas Moleculares - Instituto de Ciencias Físicas - UNAM, LEAM - ESCUELA DE QUÍMICA - UIS COLLABORATION — Fluoromethanes ($\text{CH}_n\text{F}_{4-n}$, $n=0-3$) are compounds characterized by a high reactivity. They are liberated into the atmosphere as consequence of anthropogenic activity. In the higher atmosphere, they can dissociate by the interaction with UV photons and other energetic particles. From experiments in our laboratory we had observe that these compounds dissociate when they interact with high density of photons. In this work we attempt to explain the main dissociation mechanisms involved when these molecules interact with photons of 255 and 355 nm, and the resulting products are neutral fragments with one and two atoms. The first electronic states, S_0 to S_8 and T_1 to T_8 , of above mentioned compounds were calculated using time dependent density functional theory along the C-F and C-F₂ coordinates. From theoretical results we observe that C-F dissociation channel can be easy reached by the absorption of one photon of 266 or 355 nm, leading the formation neutral F and $\text{CH}_n\text{F}_{3-n}$ ($n=1-3$). Another mechanism is a two step processes mediated by stable transition structures, the molecule can dissociate as F₂ and $\text{CH}_n\text{F}_{2-n}$ ($n=1,2$).

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