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ATMOSPHERIC POLLUTANTS; CO_2 CAPTURE

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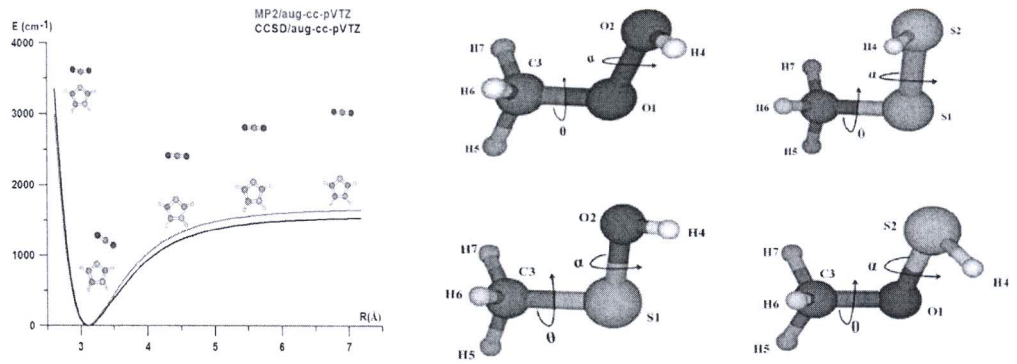
Abstract

The present-day atmosphere is quite different from the natural atmosphere that existed before the Industrial Revolution, in terms of chemical composition, if the natural atmosphere is considered to be "clean", then this means that clean air cannot be found anywhere in today's atmosphere. Many processes are responsible for atmospheric pollution. We present here several studies concerning the spectroscopy of atmospheric species such as CO_2, Methyl hydroperoxide (MHP; CH3-O-OH), Methyl hydrodisulfide (MDS; CH3-S-SH), Methane sulfenic acid (MSEA; CH3-S-OH) and methylsulfanol (CH3-O-SH). In addition, we analyze the job of CH_3, OCH_3 and SCH_3 radicals in chemical processes. We use highly correlated ab initio methods for these studies.



CH_3-X-YH (X, Y=O,S) are not well characterized species. Thus, we present a complete ab initio study concerning structure and spectroscopic properties. This study takes into consideration the non-rigidity. The radicals CH_3, OCH_3 and SCH_3 are products of the chemical decomposition of many pollutants. Their processes involve many electronic states.

Carbon dioxide, a well known species, is considered the main cause of climate change. Indeed, it is the principal rejected by the chemical industry and the exhaust gas carbon compound. For these reasons, we are interested in several intramolecular processes relevant for CO_2 capture. Potential Energy Surfaces (PES) describing the interaction between imidazole and CO_2 are explored for been used in solid-state simulations. Imidazole is a relevant building block of Zinc Imidazolate Frameworks (ZIFs) a group of Metal Organic Frameworks (MOFs) recently proposed in the field as potentially interesting materials for CO_2 adsorption and separation purposes. PES are calculated using CCSD(T)-F12 techniques, this is done in further work on the substituted imidazoles (M.Salah et al.).