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"Photoionization and photofragmentation of substituted organic molecules"

Abstract

The abundance and relevance of organic molecules similar to benzene makes their study important. Studying the interactions of such molecules with intense light fields has implications for the generation of short-wavelength radiation, attosecond science, high-harmonic generation, and many other fields. However, the computing power necessary to complete fully *ab initio* calculations describing the dynamics of molecules of this size does not exist, which makes experimental observations even more important.

Since many organic molecules are similar, it is possible to construct systematic series which differ from each other by a single structural parameter. Any differences in the intense-field behaviors between two molecules in such a series must then be a result of the structural parameter which is different. Our experiments, which avoid the focal volume effect, are sensitive to the dynamics of photoionization and photofragmentation process which result from interacting molecules in the gas phase with ultrafast (50 fs, 800 nm) laser pulses.

Results will be presented for three primary series of molecules. The halobenzenes substitute a hydrogen atom from the benzene structure for a halogen atom; within this series the substituents are progressively heavier, and substituent size is the controlling factor in the dynamics. Similarly, the C-N-O-F isoelectronic series replaces a hydrogen atom with methyl (–CH_3), amine (–NH_2), and hydroxyl (–OH) groups, as well as atomic fluorine. These substituents are isoelectronic and represent different functional substitutions with similar size. Also considered are compound substitutions such as the methoxyl group (–O–CH_3), and a comparison between amine (–NH_2) and nitro (–NO_2) substitutions. Finally, the azabenzenes are studied, which involve replacing one or more C–H units with a nitrogen atom. Effects of symmetry are considered for pyridine (azabenzenes), pyridazine (1,2-diazine), pyrimidine (1,3-diazine), and pyrazine (1,4-diazine).