STRUCTURE DETERMINATION OF NON-LINEAR HYDROCARBON CHAINS BY DEUTERIUM LABELING

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Isotopic labeling is an analytical tool that has been widely used in chemistry and biochemistry. In this contribution, we illustrate the potential of isotopic labeling in the structure determination of gaseous carbon-chain radicals. More spefically, systematic deuterium labeling experiments are presented for three non-linear hydrocarbon chains (C_9H_3 with C_{2v} symmetry, and two $C_{11}H_3$ isomers with C_{2v} and C_s symmetries, respectively), where the H/D atoms in these molecules are chosen as isotopic tracers.[a] In the experiment, electronic absorption spectra are recorded for these target hydrocarbon chains and their (partially) deuterated equivalents in special hydrocarbon plasma expansions constituting C/H, C/D, and C/H/D, respectively. The number of observed bands, the quantitative determination of isotopic shifts, and supporting DFT-calculations make it possible to unambiguously identify the geometric structures of HC_4CHC_4H, $HC_4C(C_2H)C_4H$, and HC_4CHC_6H. This result also confirms that optical spectra of D-substituted species can provide molecular symmetry information of polyhydrides, as well as chemical bond correlations in the substructures containing D-labeled hydrogen. Deuterium labeling, therefore, is considered as a useful approach to characterize the molecular structure of gaseous hydrocarbons.

[a] D. Zhao, H. Linnartz, W. Ubachs *J. Chem. Phys.* **136**(5), 054307 2012; and D. Zhao, M. A. Haddad, H. Linnartz, W. Ubachs *J. Chem. Phys.* **135**(7), 074201 2011.