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Generation of polyyne and methylpolyyne molecules from toluene by intense femtosecond laser pulse irradiation

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Synopsis Hydrogen-capped and methyl-capped carbon chains (polyynes) have been generated by intense femtosecond laser irradiation of pure liquid toluene. UV-Vis and Raman spectroscopy were used to confirm the presence of polyynes in the irradiated samples, and high performance liquid chromatography (HPLC) was used to separate polyynes up to $C_{18}H_2$ and $HC_{13}CH_3$.

Polyynes are linear carbon chain clusters with an even number of carbon atoms alternating triple and single sp-hybridized C–C bonds, usually terminated by hydrogen atoms. They have been detected in the interstellar medium, and could be important precursor molecular components in the formation of fullerenes and carbon nano-tubes [1]. Polyynes have been used as nano-conductors and can form novel coaxial nano-wires by insertion into single wall carbon nano-tubes.

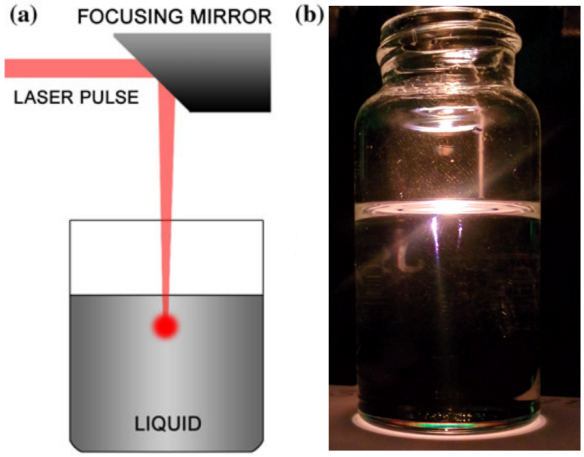

Figure 1. (**a**) A schematic of the experimental setup. (**b**) An image of the laser-liquid interaction during irradiation.

Toluene in small vials was irradiated by 100 fs pulses from a 240 μJ regeneratively amplified Ti:Sapphire tabletop laser with a 1 kHz repetition rate and central wavelength of 800 nm. The irradiation time was varied between 1-4 hours. A schematic of the irradiation setup is shown in Fig. (1a). The laser beam was focused directly below the meniscus of the liquid using a 50 mm focal length mirror. Consequently, a very intense ($> 10^{13}$ W/cm2), highly luminous, dissociation and ionization region formed, as shown in Fig. (1b).

After irradiation, Raman spectroscopy was performed on irradiated samples, indicating the presence of polyynes as large as $C_{20}H_2$ when compared to density functional simulations [2]. Fig. 2 shows that HPLC confirms the presence of polyynes up to $C_{18}H_2$ and $HC_{12}CH_3$. Hexane experiments suggest that formation via single step rearrangement of the parent molecule is not likely [3]. Formation mechanisms will be discussed including the significance of laser filamentation.

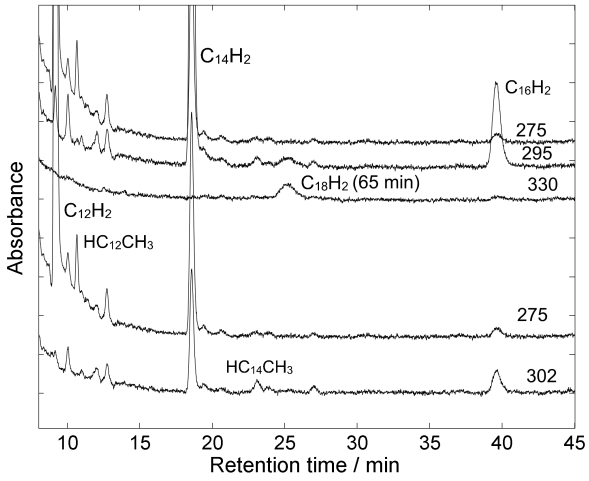

Figure 2. Analytical HPLC chromatograms of the irradiated samples, each labelled on the extreme right by its corresponding absorption wavelength in nm.

References

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