

Investigation of the H- (D-) loss from toluene's isotopologues in the fs timescale

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The H-loss (or D-loss from the deuterated isotopologues) is the primary dissociation channel of toluene ($C_6H_5CH_3$). This dissociation channel is related to the radical [P-H] (P stands for the parent molecule) photo-isomerization, i.e. the six-membered (benzyl) to a seven-membered (troyl) ring isomerization. The dynamics of this channel is studied in the fs timescale using a pump/probe excitation scheme in conjunction with a time-of-flight mass spectrometer. The 5th harmonic of a Ti:Sapphire femtosecond laser (160 nm) is used as the pump beam and a part of the fundamental laser beam (800 nm) serves as the probe. Three isotopologues of toluene have been studied ($C_6H_5CH_3$, $C_6H_5CD_3$, $C_6D_5CD_3$). The dependence of the H- and D-loss on the delay time between the pump and the probe beams is presented for the first time. Furthermore, the influence of the isotopic effect versus that of the H-scrambling (Fig. ??), which attracted the researchers' interest in the past [1], is discussed.

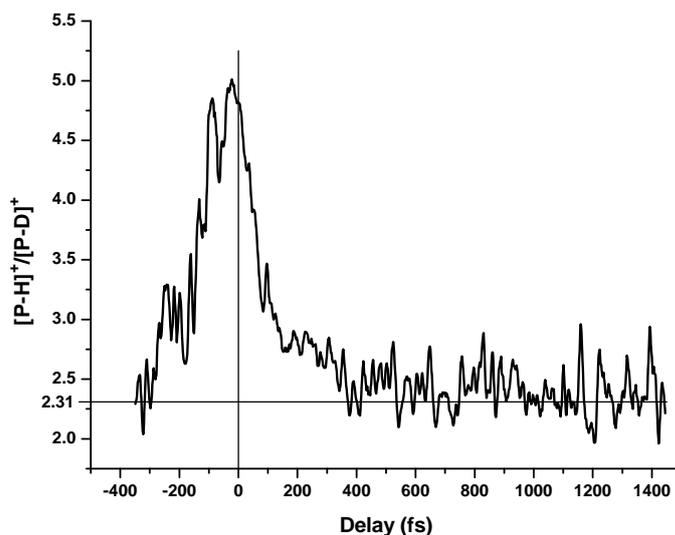


Figure 1: $[H-loss]/[D-loss]$ channel ratio in the case of $C_6H_5CD_3$.

Acknowledgements

We would like to thank Dr. E. M. Bennis for his contribution in the development of the experimental setup.

This research has been co-financed by the European Union (European Social Fund – ESF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: **THALES (ISEPUMA)**. Investing in knowledge society through the European Social Fund.

References

[1] T. A. Field *et al.* Chem. Phys. **250**, 81–110 (1999)