

Abstract Submitted
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Resonant photodissociation in substituted benzenes¹ TIM SCARBOROUGH, COLLIN MCACY, DAVID FOOTE, CORNELIS UITERWAAL, University of Nebraska - Lincoln — Cyclic aromatic molecules are abundant in organic chemistry, with a wide variety of applications, including pharmacology, pollution studies and genetic research. Among the simplest of these molecules is benzene (C₆H₆), with many relevant molecules being benzene-like with a single atomic substitution. In such a substitution, the substituent determines a characteristic perturbation of the electronic structure of the molecule. We discuss the substitution of halogens into the ring (C₆H₅X), and its effects on the dynamics of ionization and dissociation of the molecule without the focal volume effect [1]. In particular, using 800-nm, 50-fs laser pulses, we present results in the dissociation of fluorobenzene, chlorobenzene, bromobenzene and iodobenzene into the phenyl ring (C₆H₅) and the atomic halogen, and the subsequent ionization of these fragments. The impact of the “heavy atom effect” on a $^1(\pi,\pi^*) \rightarrow ^3(n,\sigma^*)$ singlet-triplet intersystem crossing will be emphasized. Currently under investigation is whether such a dissociation can be treated as an effective source of the neutral substituent.

[1] J. Strohaber and C. Uiterwaal, Phys. Rev. Lett. **100** 023002 (2008).

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