Abstract Submitted
for the DAMOP15 Meeting of
The American Physical Society

Collisions induced dissociation and Ab initio study of azobenzene derivatives bond structure and electronic configuration MOHAMMADREZA REZAEE, Physics and Astronomy Department, University of Tennessee, Knoxville, ROBERT COMPTON, Physics and Astronomy Department, Department of Chemistry, University of Tennessee, Knoxville — Collision induced dissociation (CID) and ab initio calculations were utilized to study a few derivatives of azobenzene molecule and their product ions. High level computational methods along with large basis set size yield values in close agreement with the experimental results. Möller-Plesset and coupled-cluster theory including perturbative triple excitations, CCSD(T), method were performed to obtain a high accuracy estimation of the bond dissociation energy value. The electron affinities have been studied experimentally using the photoelectron spectroscopy method as well as theoretically using ab inito calculations. For the trans-2,2',6,6' tetra-fluoro azobenzene the bond dissociation has been experimentally determined to be 1.88 eV and the vertical detachment energy is 1.78 eV.

Mohammadreza Rezaee
Physics and Astronomy, University of Tennessee, Knoxville

Date submitted: 29 Jan 2015 Electronic form version 1.4