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**Collision induced dissociation study of azobenzene and its derivatives: computational and experimental results** MOHAMMADREZA REZAEE[1], ROBERT COMPTON[2], University of Tennessee, Knoxville — Experimental and computational investigation have been performed in order to study the bond dissociation energy of azobenzene and its derivatives using collision induced dissociation method as well as other energy and structural characteristics. The results have been verified by comparing with results obtained from computational quantum chemistry. We used different density functional methods as well as the Möller-Plesset perturbation theory and the coupled cluster methods to explore geometric, electronic and the spectral properties of the sample molecules. Geometries were calculated and optimized using the 6-311++G(2d,2p) basis set and the B3LYP level of theory and these optimized structures have been subjected to the frequency calculations to obtain thermochemical properties by means of different density functional, Möller-Plesset, and coupled cluster theories to obtain a high accuracy estimation of the bond dissociation energy value. The results from experiments and the results obtained from computational thermochemistry are in close agreement.

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