

Double photoionization of tribromoborazine

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Synopsis We have measured the relative double photoionization yield of tribromoborazine [(BrBNH)₃], which has the same molecular structure as benzene. We compare the photon-energy dependence of the double-photoionization process for these two molecules.

In previous investigations on the double photoionization of aromatic molecules [1] it was found that the ratio of doubly to singly charged parent ions exhibits a photon-energy dependence that is similar to the one for the ratio of doubly to singly charged helium ions at low energies. Towards higher photon energies this ratio increases linearly for aromatic molecules but not for atoms and molecular nitrogen [2]. In addition, aromatic molecules with a hexagonal ring structure, such as benzene, show a broad resonant enhancement of the ratio (“hump”), which was interpreted as the result of the formation of a two-electron pseudoparticle [3] that has a de Broglie wavelength that matches approximately the C-C distance in the molecule such that the wave forms a closed loop.

Here we present results on the double photoionization of tribromoborazine [(BrBNH)₃], which has the same molecular structure as benzene but is not aromatic (nor even organic). How similar is the ratio of doubly to singly charged parent ions for these two molecules?

We have performed ion time-of-flight measurements on the VLS-PGM undulator beamline [4] at the Canadian Light Source using photons from 25 to 138 eV. The photons entered the chamber intersecting an effusive beam of the sample gas. Electrons extracted from the interaction region served as the start pulse for the flight-time measurements.

We have found in this investigation that the ratio of doubly charged parent ions to the sum of doubly plus singly charged parent ions exhibits, as expected, a photon-energy dependence similar to helium at energies below 95 eV (see Fig. 1). At higher energies the ratio rises linearly with increasing energy — an effect that has

not been observed before for non-aromatic molecules.

We conclude that aromaticity is not required for a linear increase of the ratio. We did not observe a resonant enhancement in the ratio, which was present in the case of benzene (and some other aromatic molecules). This absence of the resonance demonstrates that aromaticity is more important than the structure of the molecule for the formation of a two-electron pseudoparticle, i.e., the π orbital in aromatic molecules is necessary for this resonance.

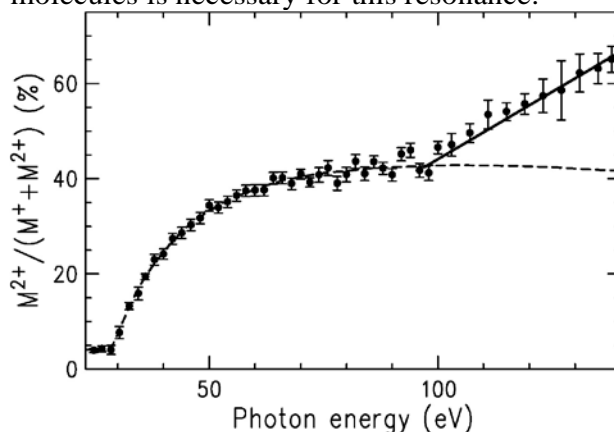


Figure 1. Ratio of doubly charged parent ions (M^{2+}) to the sum of doubly plus singly charged parent ions ($M^+ + M^{2+}$). The dashed line is a fit to the low energy data using the double-to-total photoionization ratio of He.

References

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