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UV spectroscopy of cold aromatic molecular systems as a diagnostic of size, functional group, and charge effects.

Tuesday 4 June 2019 16:15 (30 minutes)

The goal of our recent work is to determine the influence upon the fundamental physical properties of aromatic systems of various factors, notably the role of molecular size, heteroatoms, chemical functionalisation (amino, carbonyl, etc), and charge upon the molecule's optical properties. These questions are addressed by performing electronic spectroscopy and mass spectrometry on functionalised polycyclic aromatic hydrocarbon (PAH) molecules in varying charge states in a cryogenically-cooled ion trap. Experiments are supported by calculations of ground and excited state geometries and energetics.
We illustrate the principle of our combined experimental and theoretical studies using examples of simple functionalised PAHs, from which we derive general laws that can subsequently be applied to larger molecules. This approach allows us to predict the optical properties of molecules too large to study experimentally and/or theoretically.

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