Resonances in low-energy electron scattering from *para*-Benzoquinone

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Synopsis We have studied elastic and inelastic electron collisions with para-benzoquinone using the R-matrix method. We investigate all shape, mixed character and core-excited resonances identified in the energy range 0-8 eV. The characterization of these resonances is important both for electron scattering and laser-induced photodetachment processes. We present an analysis of the resonances for the equilibrium geometry of both the neutral and bound anion states. Elastic and inelastic cross sections are also presented.

para-Benzoquinone (1,4-benzoquinone or *p*-BQ) is the prototypical member of the quinone family. These molecules are commonly found in nature and play a crucial role in electron transfer reactions in chemistry and biology, for example, in photosynthesis [1]. Among its many properties, they display antitumoral activity and participate as redox cofactors in quinoenzymes. From a practical point of view, the highly symmetric structure and absence of dipole moment of *p*-BQ make it a good target for computational studies as these features simplify calculations and reduce computational cost.

A number of studies involving anionic states of *p*-BQ have been published. Experimentally, time-resolved spectroscopy of the excited-state dynamics of the anion [2], photodetachment [3], anion fluorescence [4] and electron transmission and electron energy loss spectroscopy [5] from the neutral have been investigated. Prior theoretical work has focused on the identification and characterization of resonances, mainly low lying ones (see [6] and references therein) or for a wider range of energies [7]. Unfortunately, no consistent spectrum for the *p*-BQ resonances has emerged yet. Similarly, no electron impact cross sections have been published.

We have performed calculations for electronically elastic and inelastic electron collisions with *p*-BQ using the R-matrix method [8] for the equilibrium geometry of both the neutral and bound anion states, at the Static-Exchange plus Polarization (SEP) and Close-Coupling (CC) level. Our calculations reveal the presence of several shape and core-excited (both shape and Feshbach) resonances, as well as mixed-character ones. Some of these resonances are identified for the first time.

Figure 1 shows the electronically elastic and total (summed over all excited states included in the calculation) inelastic cross sections. Many of the resonances present in the system are visible as peaks in either of both cross sections. A detailed analysis of the resonances, their characteristics and parent states will be presented at the conference.

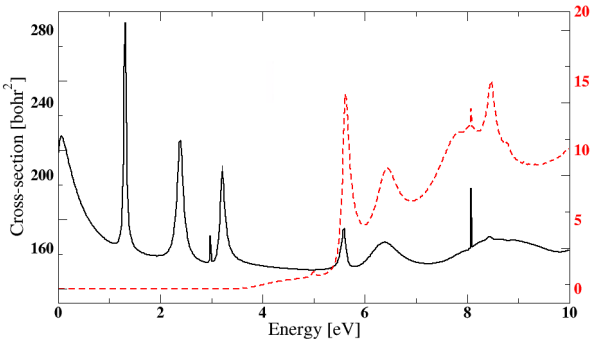

Figure 1. Total elastic (solid black line) and inelastic (dashed red line) cross sections for the ground state equilibrium geometry of *p*-BQ. Note the different scales (left and right) of the y-axis for each of the cross sections.

References

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