The absorption spectrum, mass spectrometric properties and electronic structure of ortho-benzoquinone

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Supporting information

The orthoquinone spectrum is available as an EXCEL file:
Orthoquinone Spectrum.xls

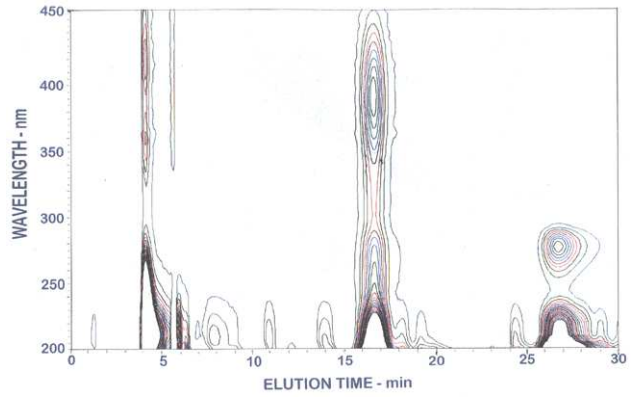

Fig. S-1 – Contour plot of a chromatographic recording fo a solution initially containing 200 μM catechol to which 1 equivalent of hexachloroiridate(IV) had been added. The signals at 4.6, 16.5 and 26.8 min represent, respectively, 200 μM hexachloroiridate(III), 100 μM orthoquinone and 100 μM catechol.

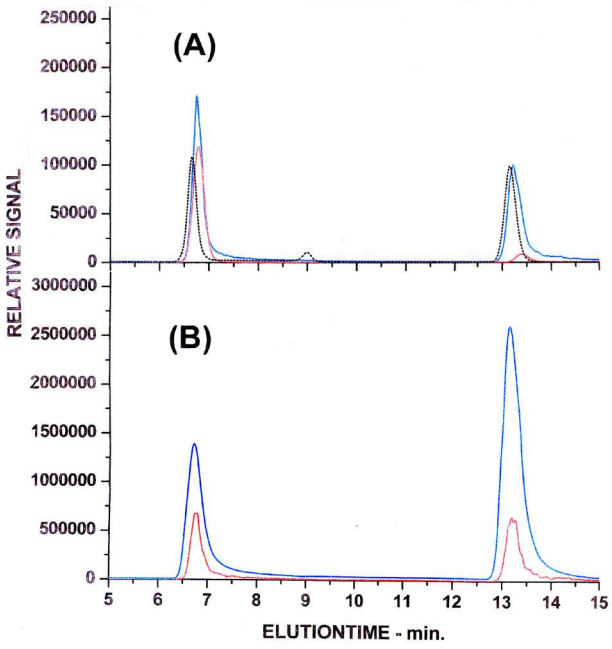

Fig. S-2 – Mass 109 chromatograms for solutions 100 uM in orthoquinone and catechol using (A) electrospray and (B) chemical ionization. **Cation** signals are in red and **anion** signals in blue. The dotted red chromatogram in A has been scaled by a factor of 10. Complementary 276 spectrophotometric data, given by the black chromatogram in A identify the mass peaks at 6.7 and 13.2 min as representing orthoquinone and catechol.

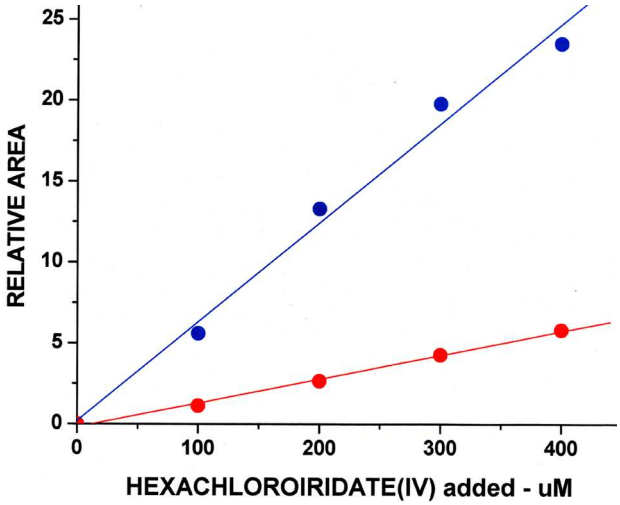

Fig. S-3 - The dependence of mass 109 cation (blue) and anion (red) signals on the concentration of hexachloroirridate(IV) added to 200 μM catechol.

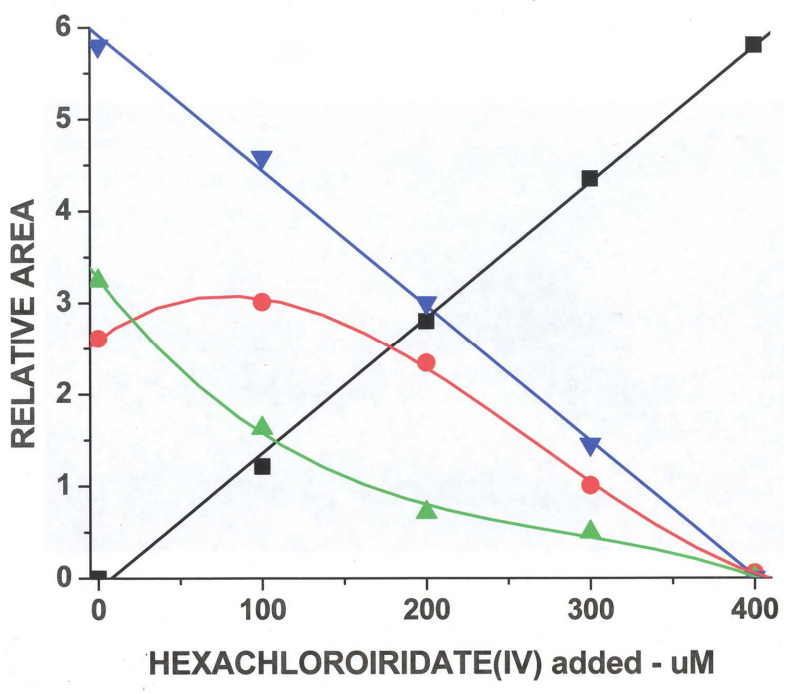

Fig. S-4 – The dependence observed in APCI experiments of the relative areas of the mass 109 **anion** signals at the orthoquinone (black) and catechol (blue) peaks on the concentration of hexachloroiridate added to 200 μM catechol. The mass 109 **cation** signal (red) at the catechol peak, however, initially increases before decreasing as the catechol is consumed. This anomalous dependence implies that using positive ion detection a non ionic intermediate. approximately indicated by the green data, is initially produced from catechol in these APCI experiments.

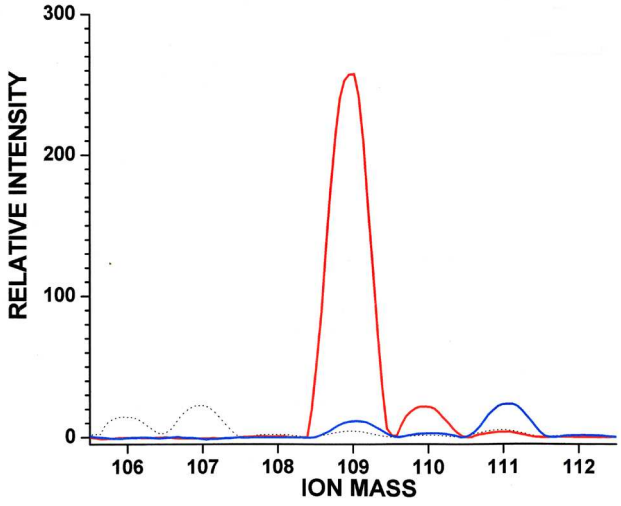

Fig. S-5 – Mass spectra recorded with the MicroMass instrument at the orthoquinone (red) and catechol (blue) peaks. The subtracted background contribution is given by the dotted spectra.

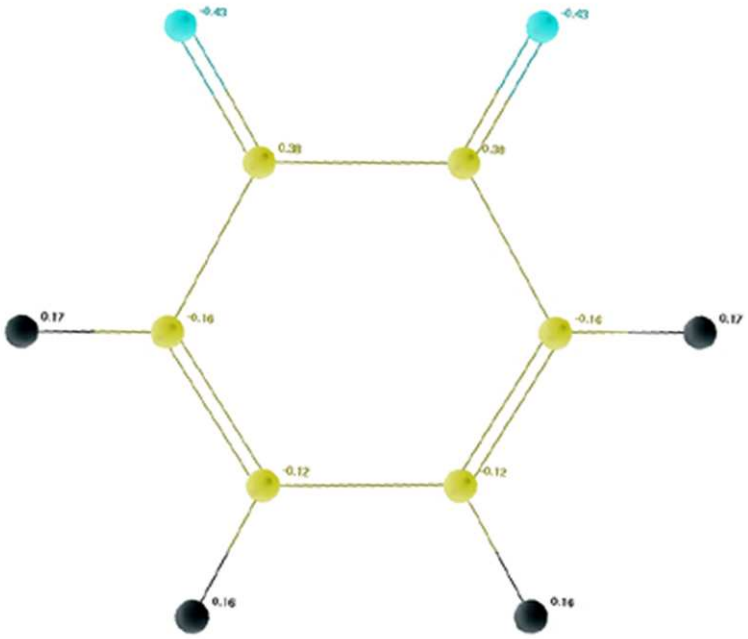

Fig. S-6 – Charge distribution in orthoquinone.

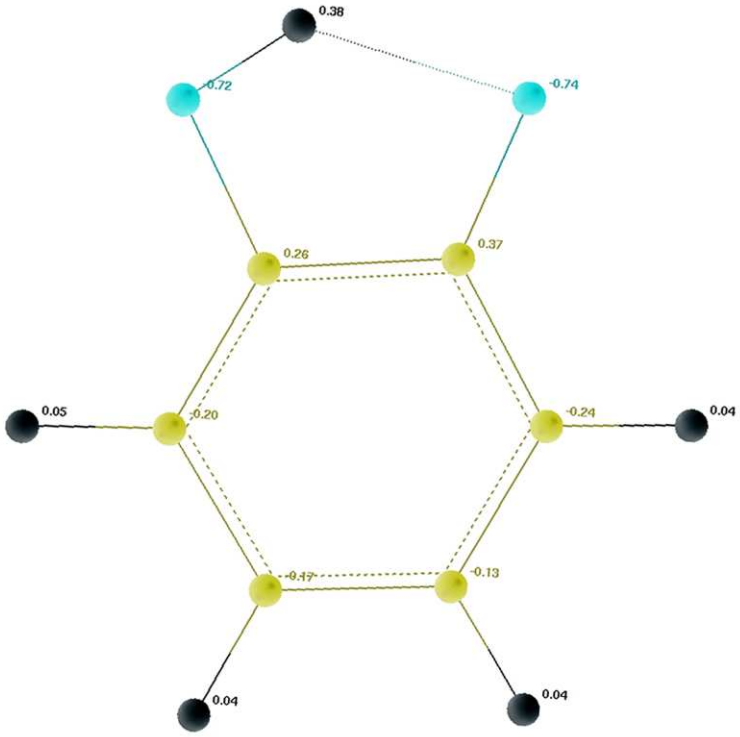

Fig. S-7 – Charge distribution in the hydride adduct at minimum energy.

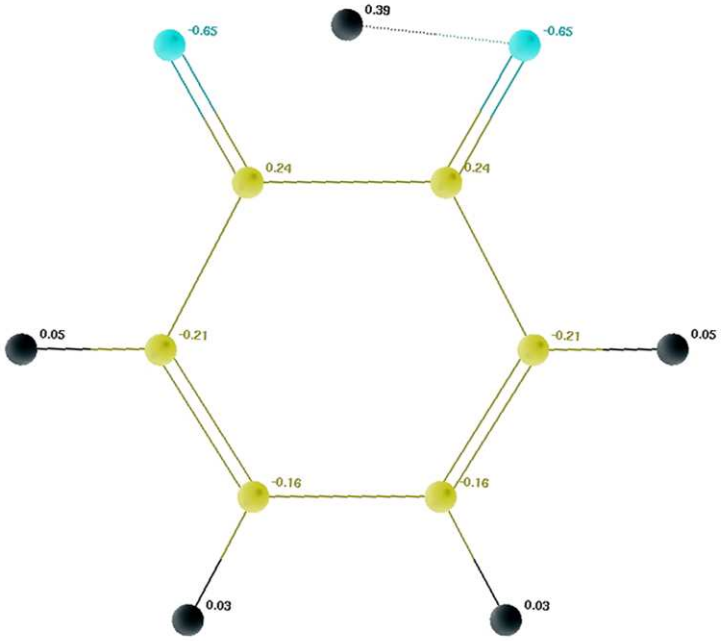

Fig. S-7T– Charge distribution in the hydride adduct at its transition state.

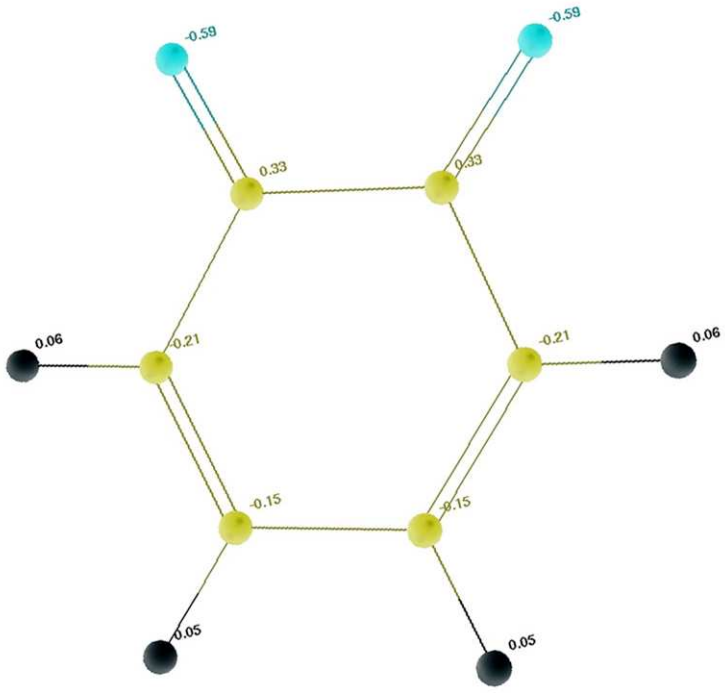

Fig. S-8 – Charge distribution in the orthosemiquinone radical anion.