## Double ionization of cycloheptatriene and the reactions of the resulting $C_7 H_n^{2+}$ dications (*n* = 6, 8) with xenon

Daniela Ascenzi,\* Julia Aysina, Emilie-Laure Zins, Detlef Schröder,\* Jan Žabka, Christian Alcaraz, Stephen D. Price, and Jana Roithová,\*

emails: ascenzi@science.unitn.it; detlef.schroeder@uochb.cas.cz; roithova@natur.cuni.cz

## **Electronic Supplementary Information**

## Content

Energy dependences of the ionic products of the reaction of $C_7 H_8^{2+}$ with neutral xenon	<b>S</b> 1
ction of mass-selected $C_7 H_6^{2+}$ with neutral xenon	S2
Reactive monitoring of mass-selected $C_7 H_6^{2+}$ with molecular nitrogen	<b>S</b> 3



**Figure S1.** Retarding potential analysis of the mass-selected  $C_7H_8^{2+}$  dication generated from dissociative electron ionization of CHT as a function of the nominal collision energy in the laboratory and of selected product ions ( $C_7H_8^+$ ,  $C_7H_7^+$ ,  $C_7H_6^+$ ,  $C_7H_5^+$ , Xe<sup>+</sup>, XeH<sup>+</sup>,  $C_7H_6Xe^{2+}$ ,  $C_6H_5^+$  and  $C_5H_3^+$ ) formed when Xe is added to the scattering cell at a pressure of about  $3 \times 10^{-3}$  mbar. The abundances are normalized (to a value of 1.0) to the largest ion intensity observed for  $C_7H_8^{2+}$  at  $E_{LAB} \sim 10$  eV. The abundances for  $C_7H_8^+$  have been corrected for isotopic <sup>13</sup>C contribution from the more intense  $C_7H_7^+$  product. Also shown is the first derivative of the retarding field curve for the primary dication.



**Figure S2.** Reaction of the mass-selected  $C_7 H_6^{2+}$  dication generated from dissociative electron ionization of CHT with Xe (at a pressure of about  $2 \times 10^{-4}$  mbar in the reaction cell) at a collision energy  $E_{CM}$ =1.1 eV. The insets a) and b) show the mass region of the Xe<sup>+</sup>/XeH<sup>+</sup> and the  $C_7 H_6 Xe^{2+}$  products on expanded scales.



**Figure S3.** Yields of the parent dications  $C_7H_6^{2+}$  (filled circles) and of the association product  $C_7H_6N_2^{2+}$  (open circles) formed in the reaction of mass-selected  $C_7H_6^{2+}$  dications with  $N_2$  as a function of the energy of photons used for the dissociative double ionization of CHT in the ion source. In the case of  $C_7H_6N_2^{2+}$  the solid line represents the data for  $C_7H_6^{2+}$  multiplied by 0.36 to indicate that the product  $C_7H_6N_2^{2+}$  appears at the same photon energy as the  $C_7H_6^{2+}$  reagent dication.