

**Supporting Information to:**

# Are the Three Hydroxyphenyl Radical Isomers Created Equal?

– The Role of the Phenoxy Radical –

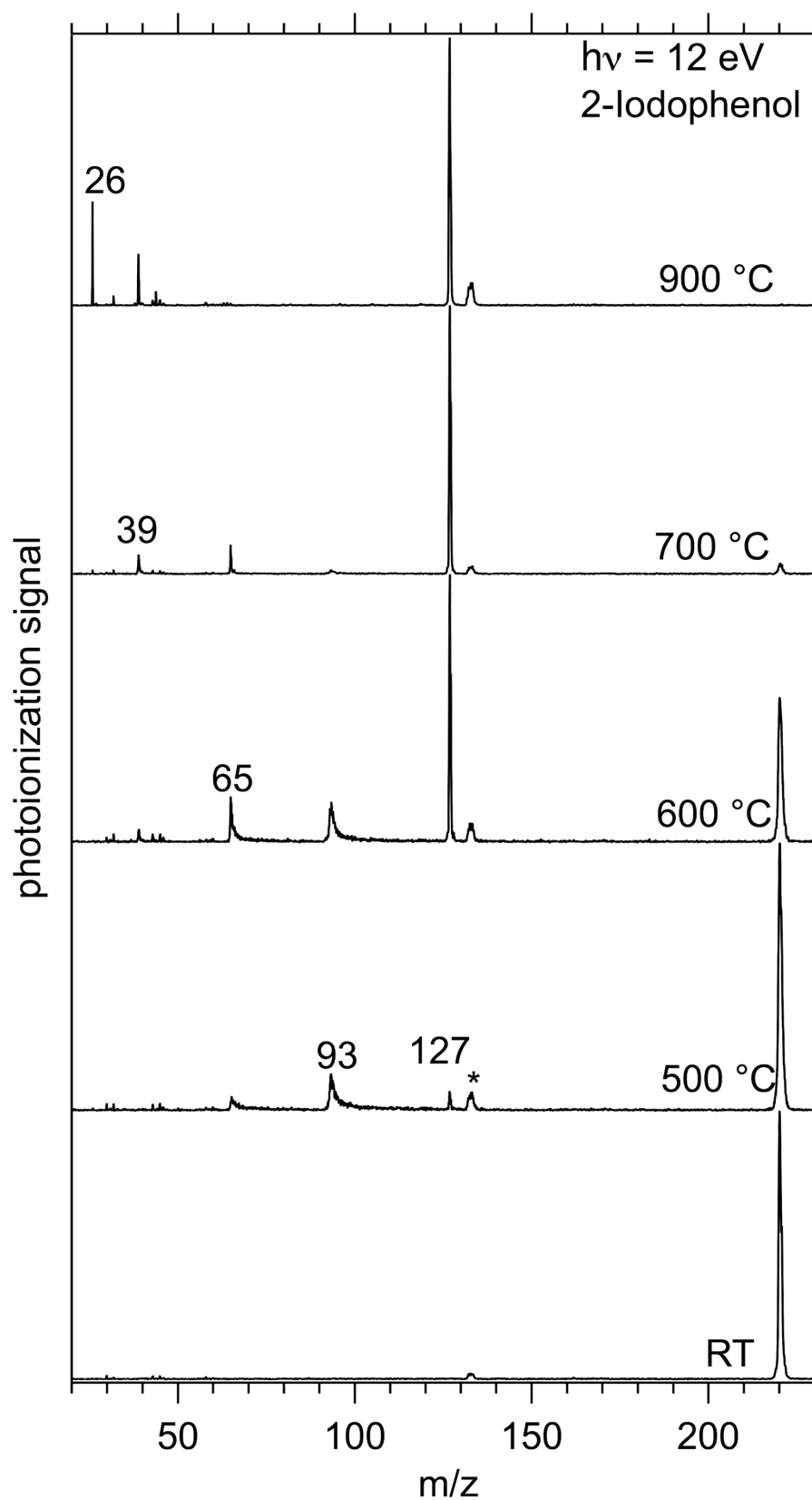
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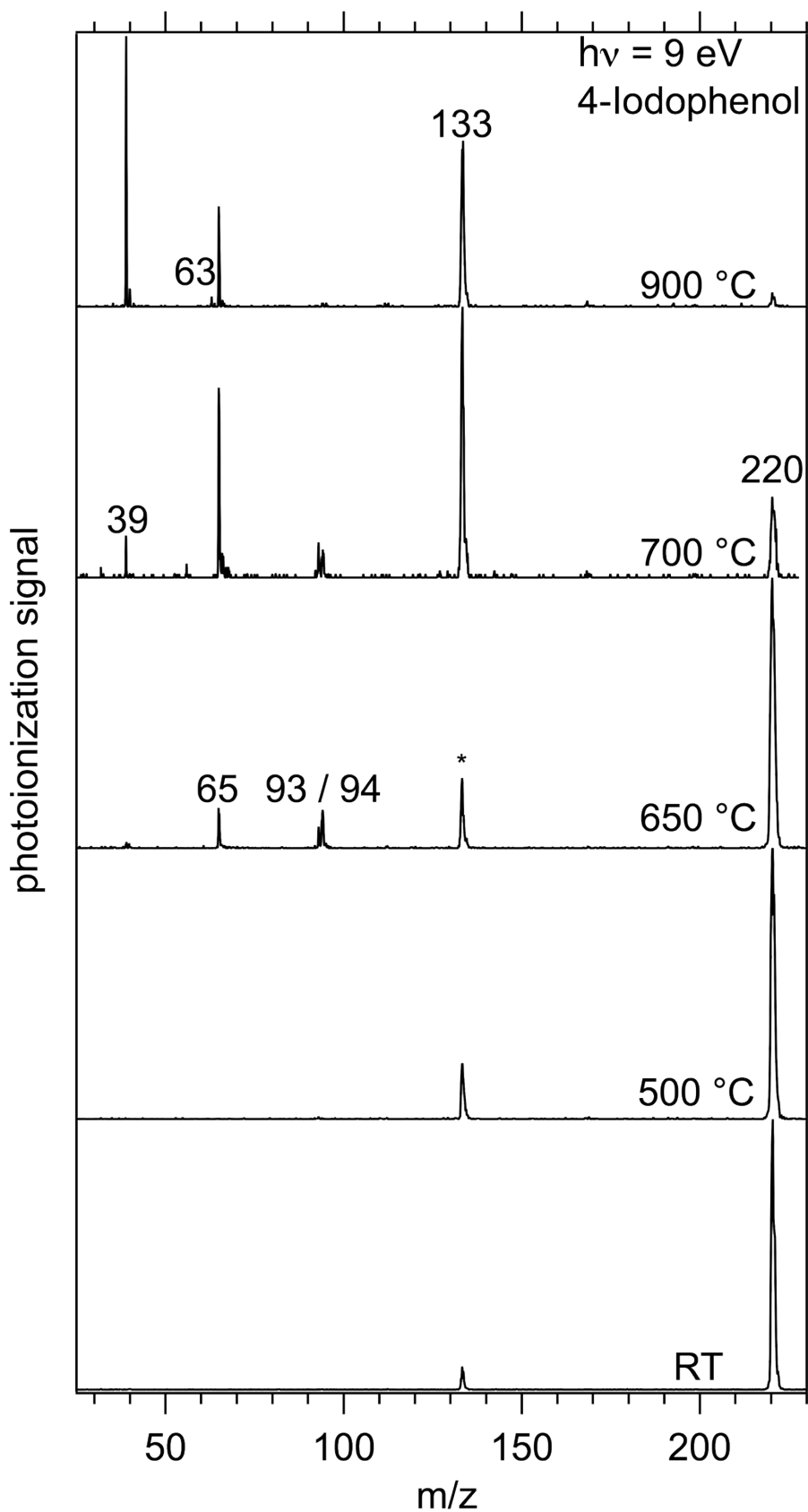
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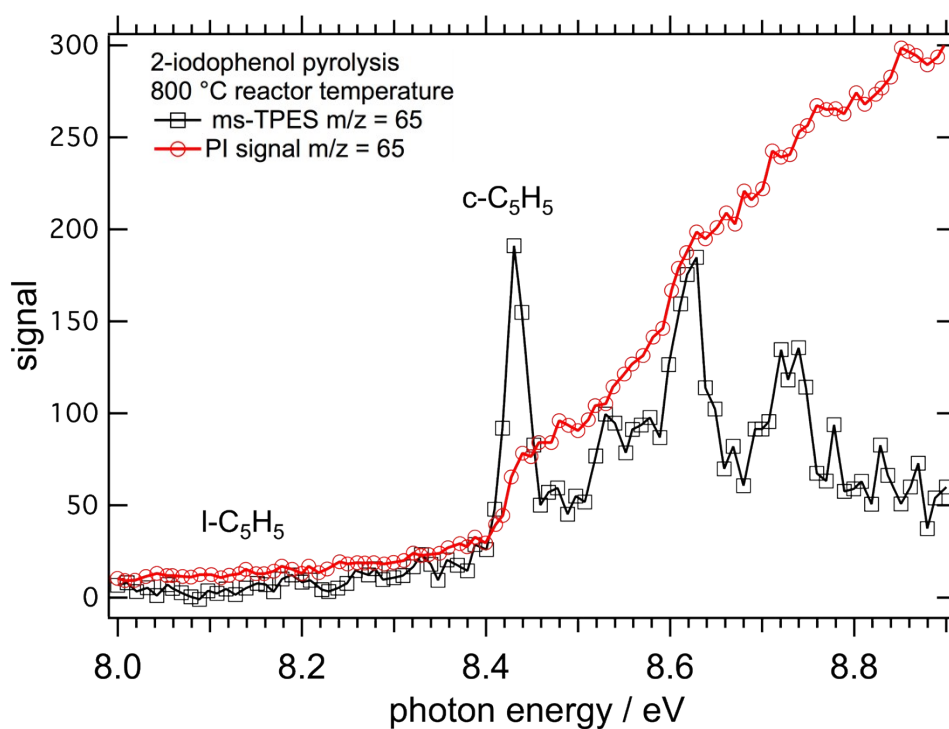
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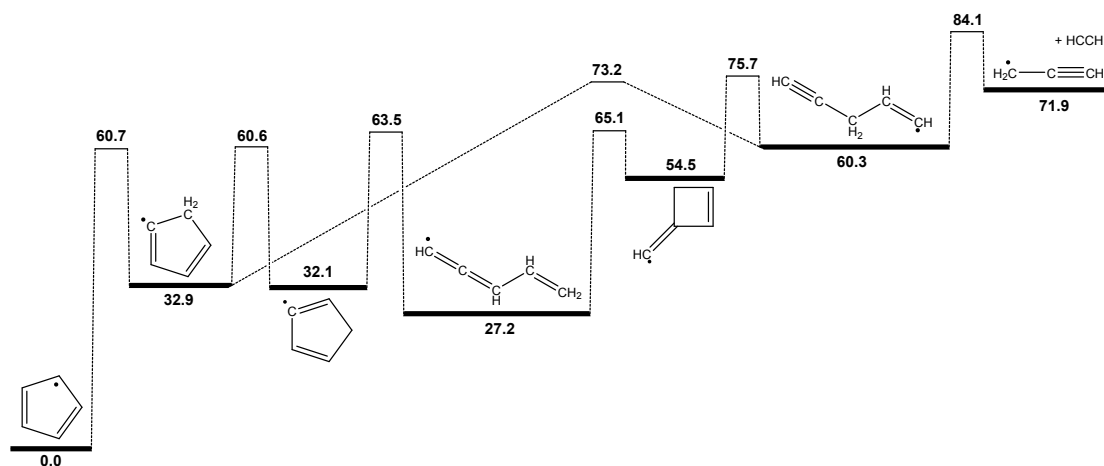
**Figure S1.** Mass spectra of 2-iodophenol as a function of the reactor temperature taken at 12 eV. Besides propargyl ( $m/z = 39$ ) we also observe the generation of acetylene ( $m/z = 26$ ), as direct decomposition product of cyclopentadienyl ( $m/z = 65$ ).  $m/z = 127$  can be assigned to iodine atoms.



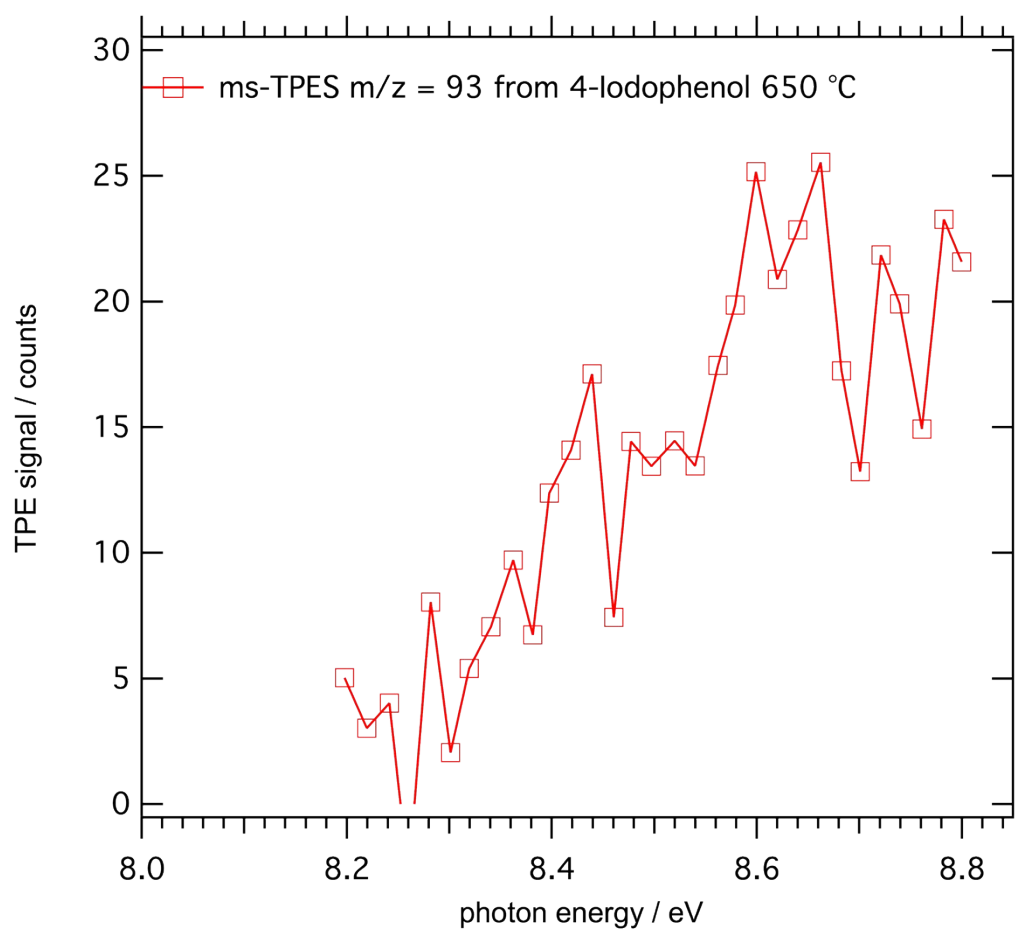
**Figure S2.** Mass spectra of 4-iodophenol as a function of the reactor temperature. The peak at  $m/z = 133$  can be assigned to 1,2,3,4- tetrahydroquinoline, which remained in the ionization chamber from previous experiments and does not affect the discussion herein. The spectra are normalized to the most intense peak.



**Figure S3.** ms-TPE and PI spectrum of  $m/z = 65$  as generated from decomposing 2-iodophenol. Besides  $c\text{-C}_5\text{H}_5$ , trace amounts of  $l\text{-C}_5\text{H}_5$  are also present, since the PI signal below 8.3 eV is not zero.



**Figure S4.** Potential energy surface showing an alternative decomposition route for  $c\text{-C}_5\text{H}_5$  proceeding via  $l\text{-C}_5\text{H}_5$  (1-vinylpropargyl) which can explain the signal below 8.2 eV in the PI or ms-TPE spectrum. G3X-K 0 K energies are shown in kcal/mol.



**Figure S5.** ms-TPE spectrum of  $m/z = 93$  derived from 4-iodophenol at 650 °C reactor temperature.