

Supporting Information to:

Are the Three Hydroxyphenyl Radical Isomers Created Equal?

– The Role of the Phenoxy Radical –

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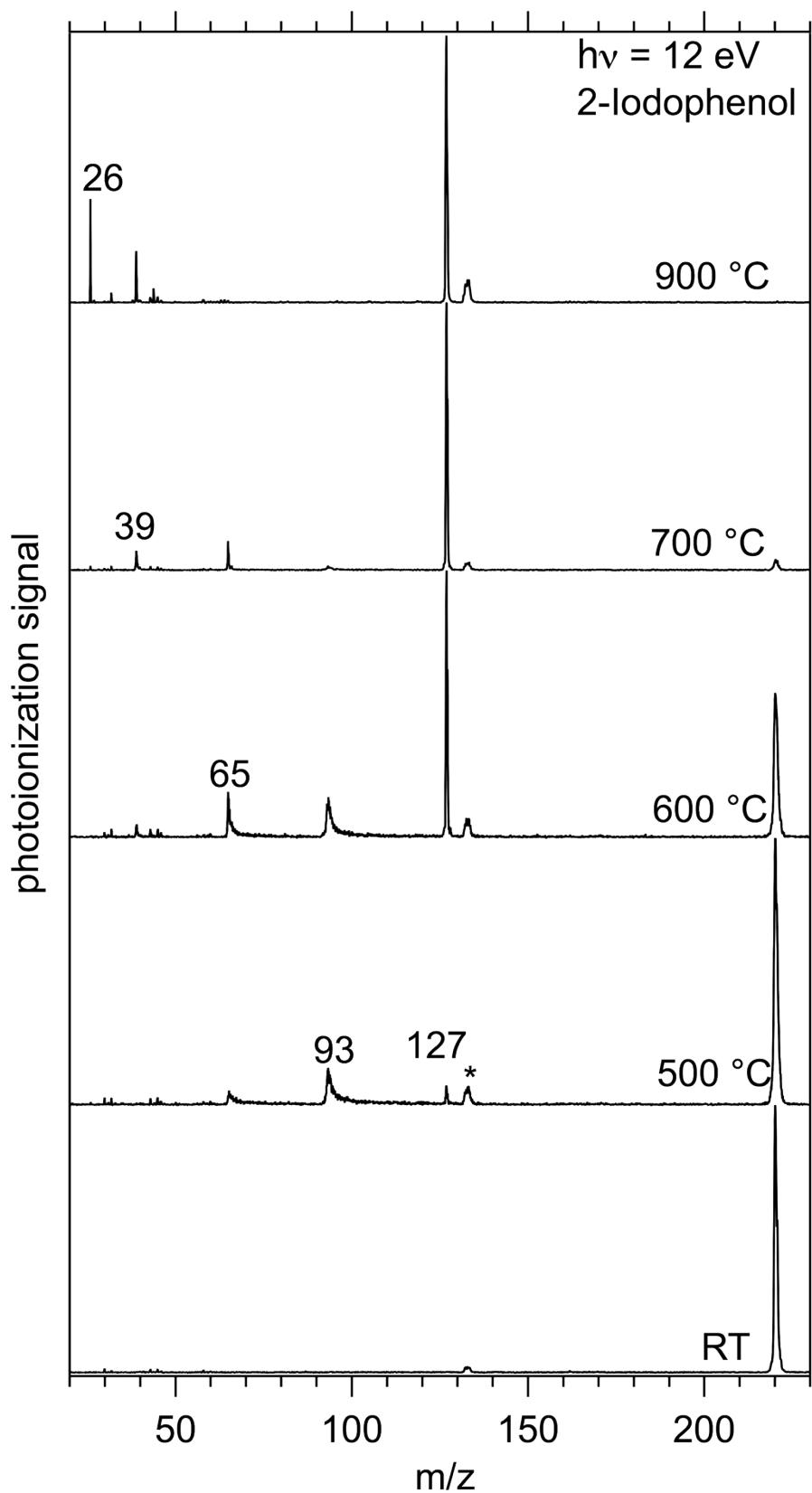


Figure S1. Mass spectra of 2-iodophenol as a function of the reactor temperature taken at 12 eV. Besides propargyl ($m/z = 39$) we also observe the generation of acetylene ($m/z = 26$), as direct decomposition product of cyclopentadienyl ($m/z = 65$). $m/z = 127$ can be assigned to iodine atoms.

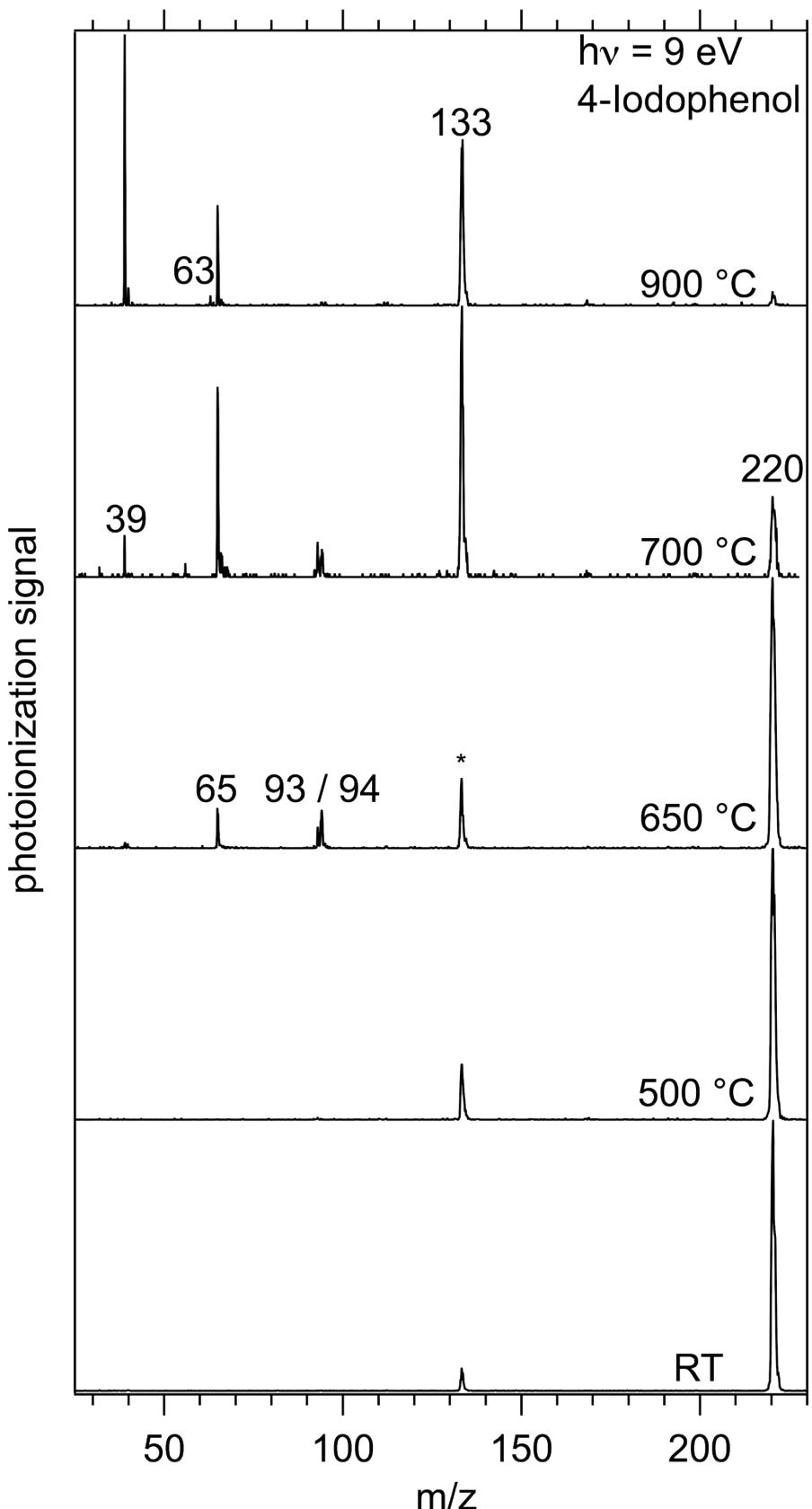


Figure S2. Mass spectra of 4-iodophenol as a function of the reactor temperature. The peak at $m/z = 133$ can be assigned to 1,2,3,4- tetrahydroquinoline, which remained in the ionization chamber from previous experiments and does not affect the discussion herein. The spectra are normalized to the most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

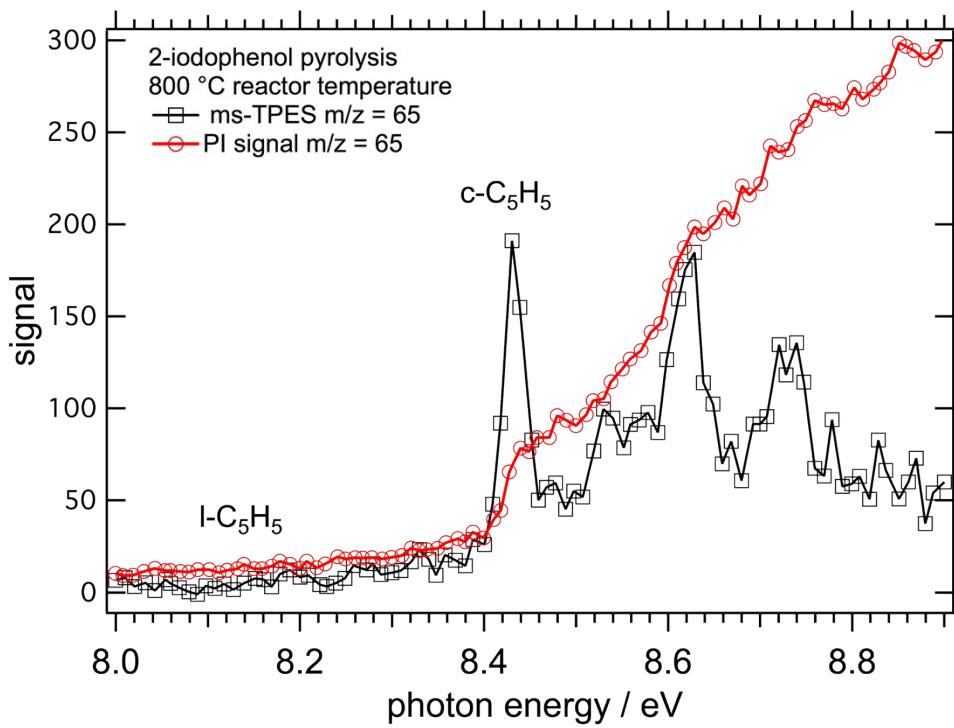


Figure S3. ms-TPE and PI spectrum of $m/z = 65$ as generated from decomposing 2-iodophenol. Besides c-C₅H₅, trace amounts of I-C₅H₅ are also present, since the PI signal below 8.3 eV is not zero.

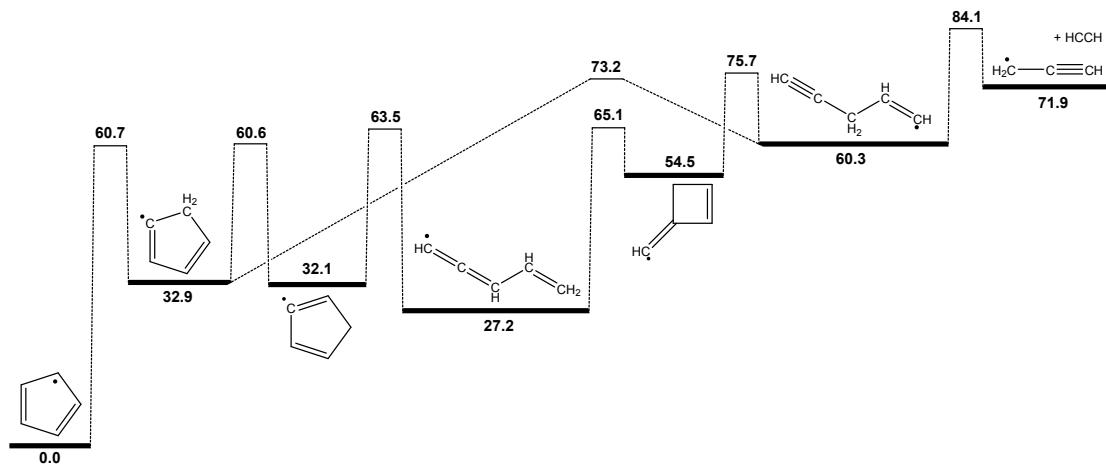


Figure S4. Potential energy surface showing an alternative decomposition route for c-C₅H₅ proceeding via I-C₅H₅ (1-vinylpropargyl) which can explain the signal below 8.2 eV in the PI or ms-TPE spectrum. G3X-K 0 K energies are shown in kcal/mol.

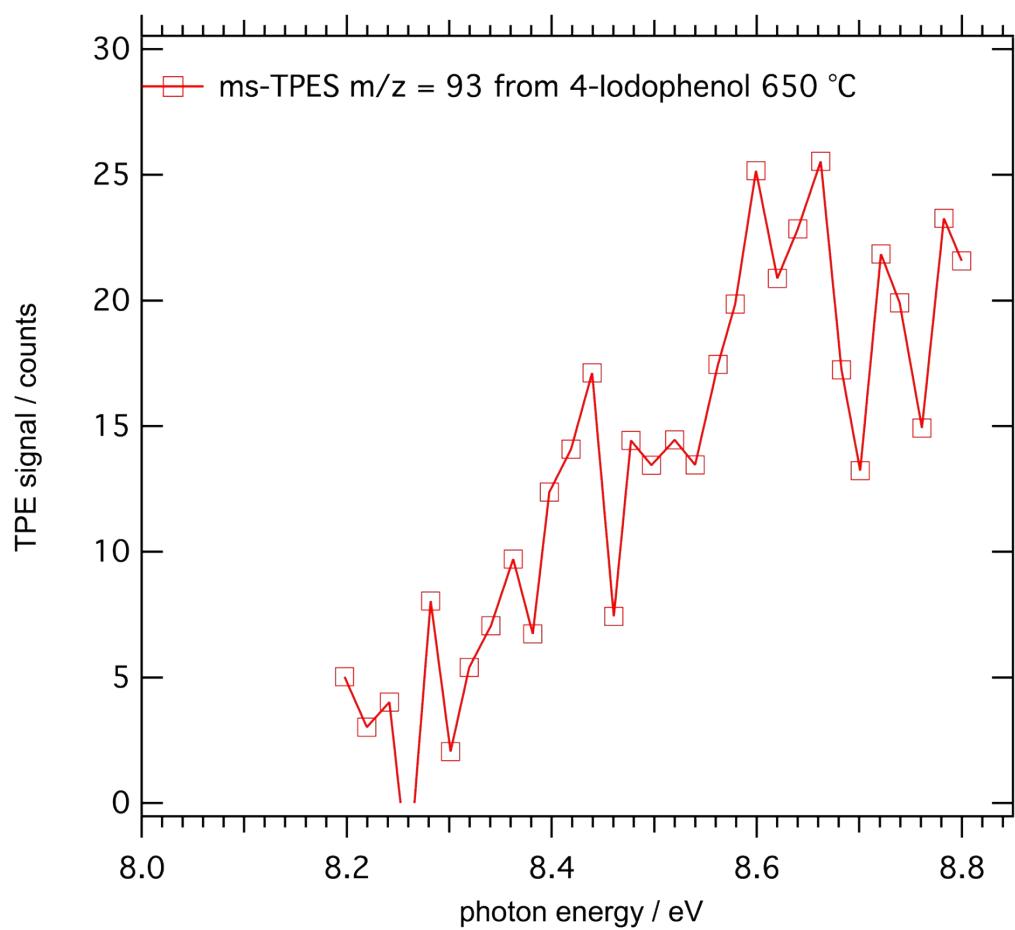


Figure S5. ms-TPE spectrum of $m/z = 93$ derived from 4-iodophenol at 650 °C reactor temperature.