Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information:

Operando PEPICO unveils the catalytic fast pyrolysis mechanism of the three methoxyphenol isomers

Zeyou Pan[a,b], Andras Bodi[a], Jeroen A. van Bokhoven[a,b], Patrick Hemberger[a]*

[a] Zeyou Pan, Andras Bodi, Jeroen A. van Bokhoven and Patrick Hemberger, Paul Scherrer Institute, 5232 Villigen, Switzerland. E-mail: patrick.hemberger@psi.ch.

[b] Zeyou Pan and Jeroen A. van Bokhoven, Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland

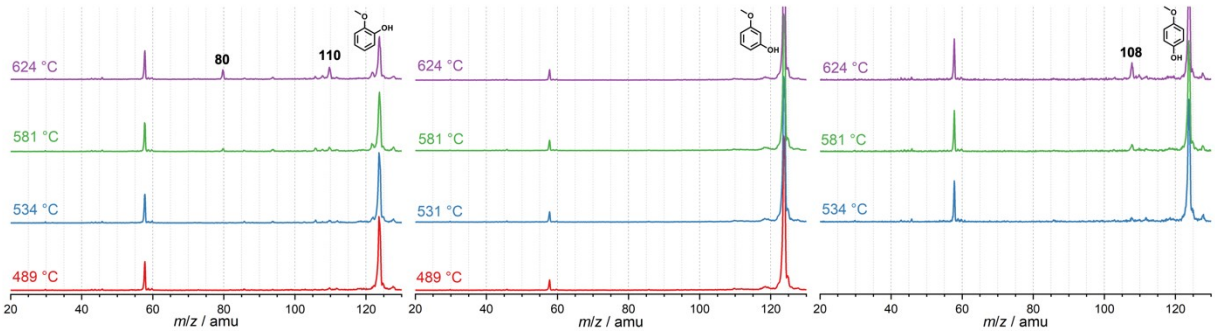

Figure S1. 1, 2-, 3- and 4-methoxyphenol pyrolysis mass spectra as function of the reactor temperature. Conditions: *hv* = 10.5 eV; ~0.01% sample in Ar; without catalyst. Only in the 2-MP and 4-MP cases could some products be observed at *m/z* 80, 110, and 108, which are assigned to cyclopentadienone, catechol and *p*-benzoquinone. The peak at *m/z* 58, acetone, is an impurity in the detection chamber and remains constant in the whole temperature range.

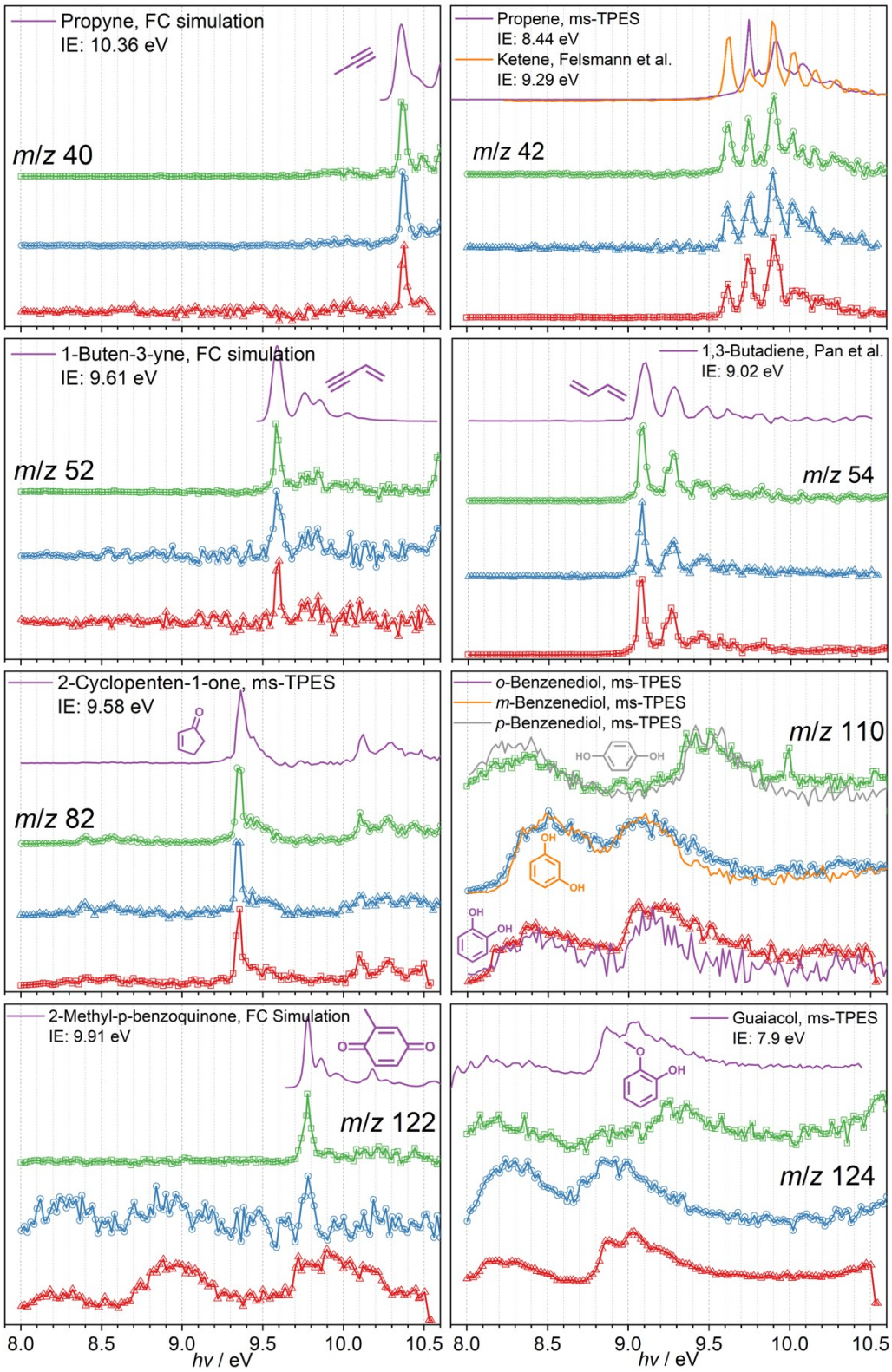

Figure S2. ms-TPE spectra of propyne (*m/z* 40), ketene[1] and propyne (*m/z* 42), vinylacetylene (*m/z* 52), butadiene (*m/z* 54)[2], cyclopentenone (*m/z* 82), the three benzenediol isomers (*m/z* 110), methyl-p-benzoquinone, and the three methoxyphenols (*m/z* 124). Red, blue, and green refer to the 2-MP, 3-MP and 4-MP catalytic pyrolysis ms-TPES over H-ZSM-5, respectively.

References:

1. D. Felsmann, K. Moshammer, J. Krüger, A. Lackner, A. Brockhinke, T. Kasper, T. Bierkandt, E. Akyildiz, N. Hansen, A. Lucassen, P. Oßwald, M. Köhler, G. A. Garcia, L. Nahon, P. Hemberger, A. Bodi, T. Gerber and K. Kohse-Höinghaus, *Proc. Combust. Inst.*, 2015, 35, 779-786.
2. Z. Pan, A. Puente-Urbina, A. Bodi, J. A. van Bokhoven and P. Hemberger, *Chem. Sci.*, 2021, 12, 3161-3169.