Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Forming a Two-Ring Polycyclic Aromatic Hydrocarbon without a Benzene Intermediate: the Reaction of Propargyl with Acetylene
DAVID OSBORN, Sandia National Laboratories, JOHN SAVEE, Los Gatos Research, TALITHA SELBY, University of Wisconsin, Washington County, OLIVER WELZ, BASF SE, CRAIG TAATJES, Sandia National Laboratories — The reaction of acetylene (HCCH) with a resonance-stabilized free radical is a commonly invoked mechanism for the generation of polycyclic aromatic hydrocarbons (PAH), which are likely precursors of soot particles in combustion. In this work, we examine the sequential addition of acetylene to the propargyl radical (H_2CCCH) at temperatures of 800 and 1000 K. Using time-resolved multiplexed photoionization mass spectrometry with tunable ionizing radiation, we identified the isomeric forms of the C_5H_5 and C_7H_7 intermediates in this reaction sequence, and confirmed that the final C_9H_8 product is the two-ring aromatic compound indene. We identified two different resonance-stabilized C_5H_5 intermediates, with different temperature dependencies. Furthermore, the C_7H_7 intermediate is the tropyl radical (c-C_7H_7), not the benzyl radical ($C_6H_5CH_2$), as is usually assumed in combustion environments. These experimental results are in general agreement with the latest electronic structure / master equation results of da Silva et al. This work shows a pathway for PAH formation that bypasses benzene / benzyl intermediates.

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Date submitted: 22 Oct 2015 Electronic form version 1.4