Scott W. Wagnon, Darshan M. A. Karwat, Margaret S. Wooldridge, Charles K. Westbrook, "Experimental and Modeling Study of Methyl *trans*-3-Hexenoate Autoignition," Energy and Fuels, dx.doi.org/10.1021/ef501806s.

Supplemental Material A: Description of the gas chromatograph systems and calibration gases.

Three GCs (Perkin Elmer Autosystem) and columns allow the stable intermediate species to be identified and quantified. GC-OHC (GC2) uses a flame ionization detector (FID) with a Varian CP-Porabond Q capillary column to target oxygenated species. GC-C5 (GC3) uses a FID with a Varian CP-Al_2O_3/Na_2SO_4 capillary column to target species smaller than C_5. GC-C10 uses a FID with a Restek RTX-1 capillary column to target species smaller than C_{10} and some oxygenated species. Helium was used as the carrier gas in all the GCs. High-purity gases were used to calibrate for methane (CH_4, Cryogenic Gases, chemically pure, 99%), ethyne (C_2H_2, Praxair, dissolved), ethane (C_2H_6, Cryogenic Gases, chemically pure, 99.0%), ethene (C_2H_4, Matheson, chemically pure, 99.5%), propane (C_3H_8, Cyrogenic Gases, instrument grade, 99.5%), propene (C_3H_6, Cryogenic Gases, polymer grade, 99.5%), and 1-butene (1-C_4H_8, Cyrogenic Gases, 99%). Calibrations were also determined using vapor from liquid methanol (CH_3OH, Sigma Aldrich, ACS spectrophotometric grade, ≥99.9%), ethanal (CH_3CHO, Fluka, puriss. p.a., anhydrous, >99.5% GC grade, ≤0.5% free acid CH_3CHO), ethanol (C_2H_5OH, Sigma Aldrich, 200 proof, anhydrous, ≥99.5%), butanal (*n*-C_4H_7OH, Sigma Aldrich, puriss., ≥99.0%), but-3-en-1-ol (C_4H_7OH, Sigma Aldrich, 96%), and methyl *trans*-3-hexenoate ($C_7H_{12}O_2$, Sigma Aldrich, 98%). Signals from the gas chromatographs were captured using a high-resolution data acquisition system (NI PXI 4472) at a rate of 8 Hz. Species were calibrated and quantified using the area under the response peak unless otherwise noted.