

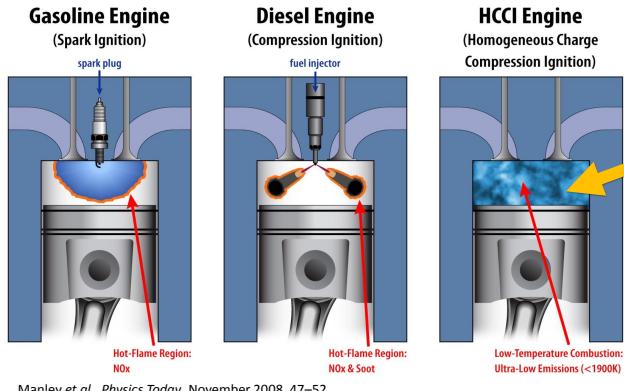
# Direct Observation and Kinetics of a Hydroperoxyalkyl Radical (QOOH)

SAND2015-2404C

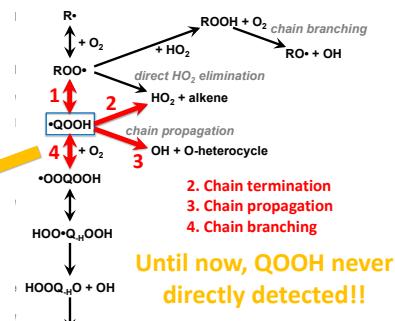
John D. Savee, Ewa Papajak, Brandon Rotavera, Haifeng Huang, Arkke J. Eskola, Oliver Welz, Leonid Sheps, Craig A. Taatjes, Judit Zádor, David L. Osborn

Four decades of research show that the QOOH intermediate plays an important role in autoignition

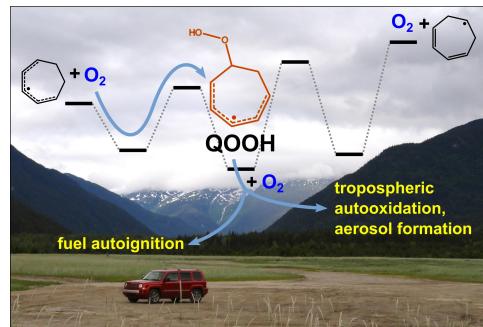
New clean efficient engine strategies depend on controlling autoignition chemistry



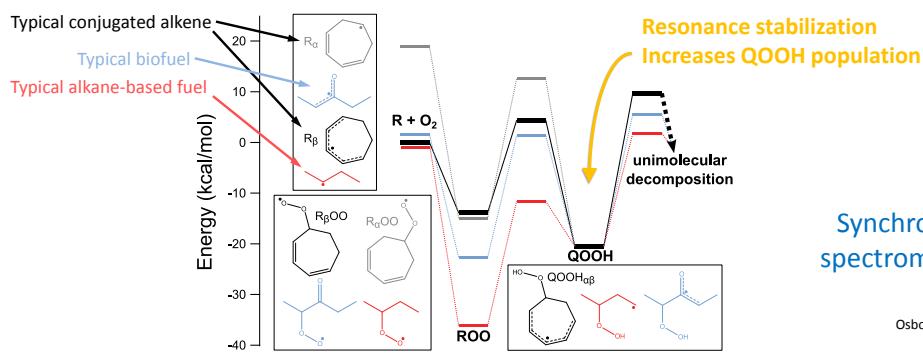
Manley et al., Physics Today, November 2008, 47-52



Autoignition and tropospheric oxidation driven by similar chemistry



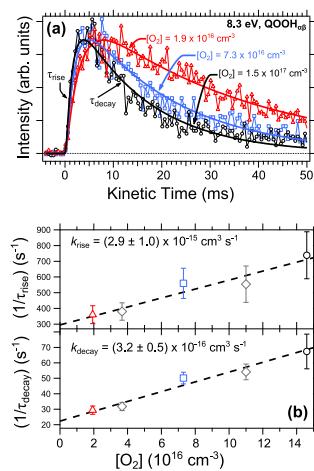
Energy landscape illustrates why QOOH is hard to detect:



Direct observation of time-dependence of QOOH yields its reactivity with O2

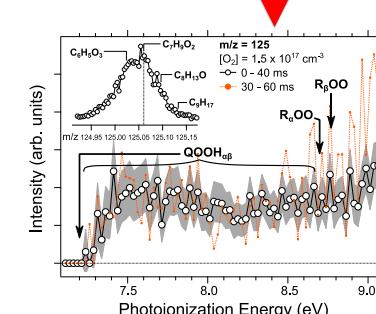
Very long QOOH lifetime due to resonance stabilization

QOOH + O2 is 10 times faster than R + O2 – will influence modeling



Direct Kinetics of R + O2 and QOOH + O2

Savee et al., Science 347, 2015, 643



ROO and QOOH have the same chemical formula (C7H9O2)  
Photoionization spectrum, exact mass, and quantum chemical calculations allow unambiguous assignment as QOOH

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