

Recent advancements in the measurements of the rate coefficients of H-abstraction by OH reactions

Aamir Farooq¹

¹*Clean Combustion Research Center, Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia
aamir.farooq@kaust.edu.sa*

Abstraction of H atoms by OH radicals is one of the most important pathways for the oxidation and breakdown of a number of compounds relevant to combustion and atmospheric chemistry. Measurements and theoretical calculations of the rate coefficients of these reactions has been the subject of many investigations over the last three decades. Depending on the structure and size of the compound, the abstraction takes place at various sites with varying rates. Most previous experimental work, however, reported the overall rate coefficients rather than site-specific rates. We have recently made several new measurements of the H-abstraction reactions for a series of important molecules and we have been able to determine the site-specific rates and branching ratios. Some of the recent work includes:

- Site-specific rate constant measurements for primary and secondary H- and D- abstraction by OH radicals: Propane and Butane. This work involved working with two normal and six deuterated alkanes to determine the site-specific rates [1].
- Site-specific rate constants and branching ratios of ketone + OH reactions. This work studied a series of small and large ketones (acetone to hexanone) to systematically determine the various abstraction pathways [2].
- Branching ratios of propene + OH reaction. Here, we studied the reaction of OH with propene and five deuterated propene isotopes to calculate the site-specific rate coefficients and branching ratios of the three abstraction channels [3].
- Reaction of OH with large alkanes. We have measured the rate coefficients of OH + alkane for eleven large alkanes. The alkanes were selected systematically to determine the site-specific rates from primary, secondary and tertiary carbons [4].
- Branching ratios of methyl ester + OH reaction. We used dimethyl carbonate to model the ester group and then determined the branching ratios of the abstraction reaction for a series of methyl esters [5].
- We have recently extended this work to study the reaction of OH with aromatic species such as xylenes and tri-methyl-benzene [6].

[1] J. Badra, E.F. Nasir, A. Farooq, *J Phys Chem A* 118 (2014) 4652-4660.

[2] J. Badra, A.E. Elwardany, A. Farooq, *PCCP* 16 (2014) 12183-12193.

[3] J. Badra, F. Khaled, B.R. Giri, A. Farooq, *PCCP* (2014) (DOI: 10.1039/c4cp04322g)

[4] J. Badra, A.E. Elwardany, A. Farooq, *Proc. Combust. Inst.* 35 (2015) (DOI: 10.1016/j.proci.2014.05.098)

[5] F. Khaled, A. Farooq, *J Phys Chem A*, submitted.

[6] A.E. Elwardany, J. Badra, A. Farooq, *Combust Flame*, submitted.