**Supplementary material**

* Exp\_IDTs.xlsx includes all the ignition delay times measured in this study.
* RCM CHEMKIN Input Files.xlsx includes all the chemkin input files needed for RCM simulations.
* The mechanism files include tmb\_nc7.inp and tmb\_nc7.dat, and the species structures are provided in species dictionary.

Some of the validation results are provided below.

# Experimental results



**Fig. S1.** Experimental and simulated results of pure 124TMB IDTs at different pressures. (a) *φ=*0.5, (b) *φ=*1.0. Solid symbols: RCM data. Solid lines: RCM simulations including facility effect.



**Fig. S2.** Experimental pressure traces of pure 124TMB RCM experiments at different temperatures.

# Validation results against experimental data in the literature





**Fig. S3.** Experimentally measured (symbols) and current model predicted (solid lines) results for 124TMB JSR data [1].



**Fig. S4.** Experimentally measured (symbols) and current model predicted (solid lines) results for 124TMB JSR data [2].



**Fig. S5.** Experimentally measured (symbols) and current model predicted (solid lines) results for *n*-heptane IDT data [3].



**Fig. S6.** Experimentally measured shock tube IDTs (symbols) and current model predicted (solid lines) results for (a) toluene [4], (b) *o*-xylene [5], (c) *p*-xylene [5].



**Fig. S7.** Experimentally measured RCM IDTs (symbols) [6] and current model predicted (solid lines) results for (a) toluene, (b) *o*-xylene, (c) *p*-xylene.

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