Supplementary material

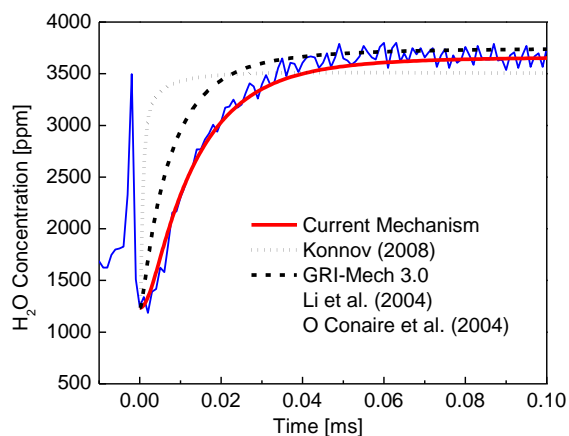

Figure S1. H_2O time-history during the thermal decomposition of H_2O_2 at 1.91 atm, 1398 K. Test mixture: 2540 ppm H_2O_2/1234 ppm H_2O/617 ppm O_2/Ar. Experimental data (in blue) from Hong et al. [16].
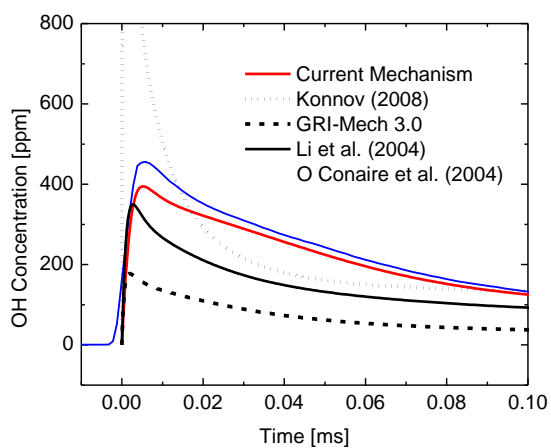

Figure S2. OH time-history during the thermal decomposition of H_2O_2 at conditions of those of Figure S1. Experimental data (in blue) are from Hong et al. [16].
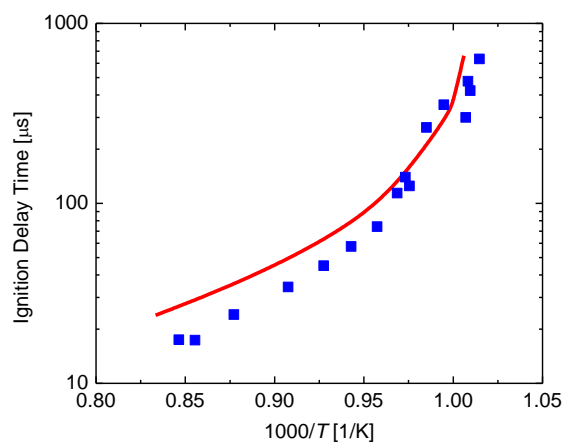
Figure S3. Comparison between experimental dat (in blue) (Slack [82]) and the prediction of the current mechanism in a stoichiometric H_2/air mixture at 2 atm.
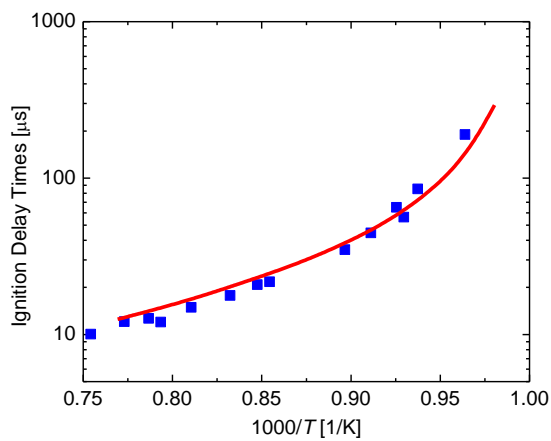

Figure S4. Comparison between experimental data (in blue) (Bhaskaran et al. [83]) and the prediction of the current mechanism in a mixture consisting of 22.59% H_2, 14.79% O_2, balance N_2 at 2.5 atm.
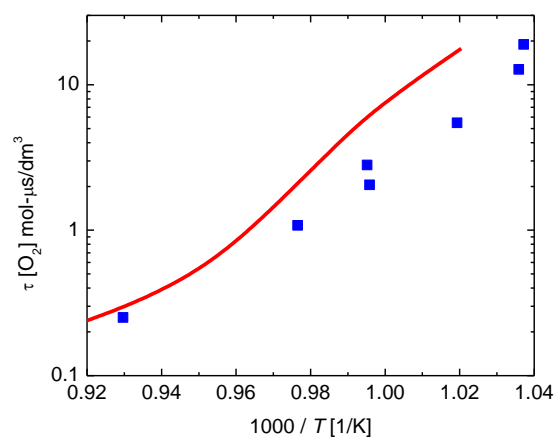
Figure S5. Comparison between experimental data (in blue) (Skinner & Ringrose [84]) and the prediction of the current mechanism in a mixture consisting of 8% H_2, 2% O_2, balance Ar at 5 atm.

Figure S6. Comparison between experimental data (in blue) (Schott & Kinsey [85]) and the prediction of the current mechanism in a mixture consisting of 1% H_2, 2% O_2, balance Ar at 1 atm.
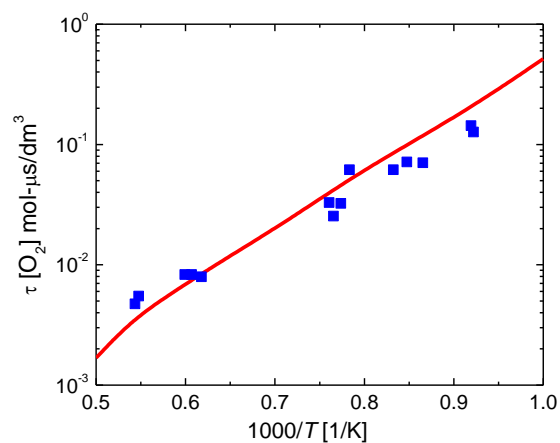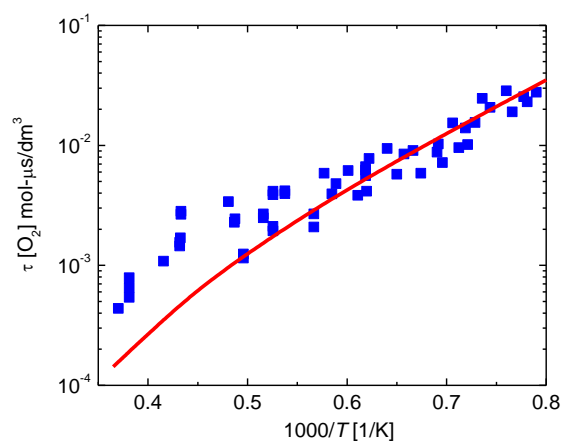
Figure S7. Comparison between experimental data (in blue) (Schott & Kinsey [85]) and the prediction of the current mechanism in a mixture consisting of 4% H_2, 2% O_2, balance Ar at 1 atm.
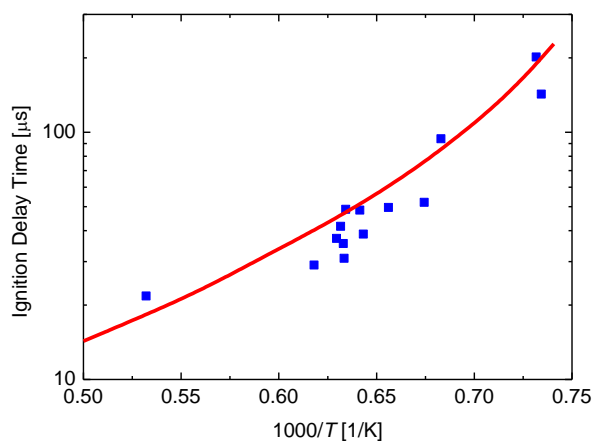

Figure S8. Experimental data (in blue) are from Petersen et al. [86]. Test mixture consisted of 0.1% H_2, 0.05% O_2, and balance Ar at 64 atm. Ignition time defined as the point where d(OH)/dt is maximum.
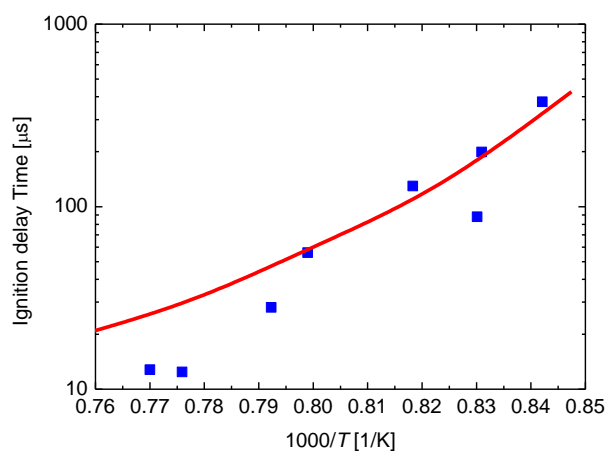
Figure S9. Experimental data (in blue) are from Petersen et al. [86]. Test mixture consisted of 2% H_2, 1% O_2, and balance Ar at 33 atm. Ignition time defined as the point where d(OH)/dt is maximum.
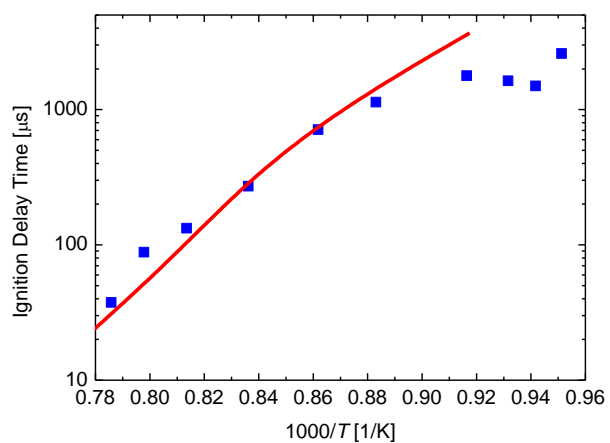

Figure S10. Experimental data (in blue) are from Wang et al. [87]. Test mixture consisted of 11.25% H_2, 63.75% air, 25% H_2O, at 4-5 atm. Ignition time defined as the onset of OH emission.

Figure S11. Experimental data (in blue) are from Wang et al. [87]. Test mixture consisted of 11.25% H_2, 63.75% air, 25% H_2O, at 9-10 atm. Ignition time defined as the onset of OH emission.
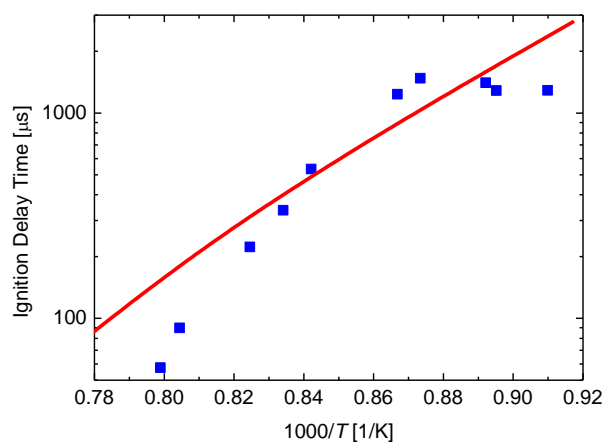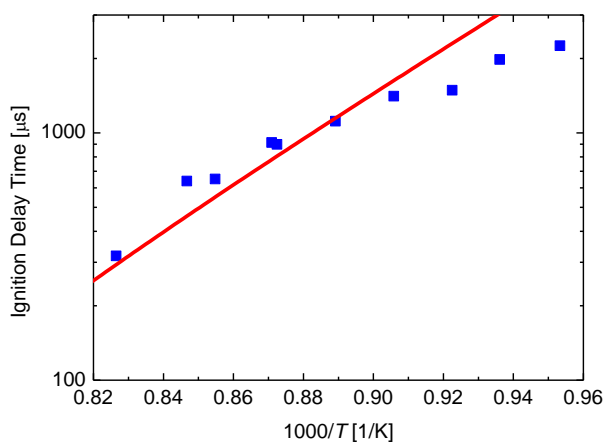

Figure S12. Experimental data (in blue) are from Wang et al. [87]. Test mixture consisted of 11.25% H_2, 63.75% air, 25% H_2O, at 15-17 atm. Ignition time defined as the onset of OH emission.
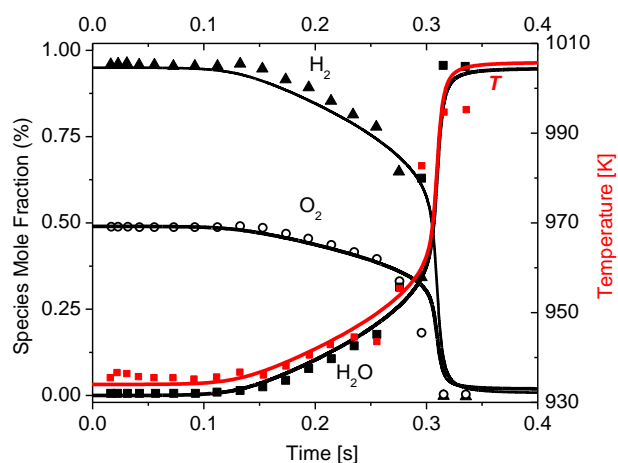
Figure S13. Species profiles from a flow reactor experiment [2]. Unburnt mixture was at 934 K, 3.02 atm and consisting of 0.95% H_2, 0.49% O_2, and N_2 balance gas. The curves are calculated with the presented mechanism by using adiabatic approximation and are shifted simultaneously by 0.22 s in time. The calculated adiabatic temperature profile is also compared with experimental values.
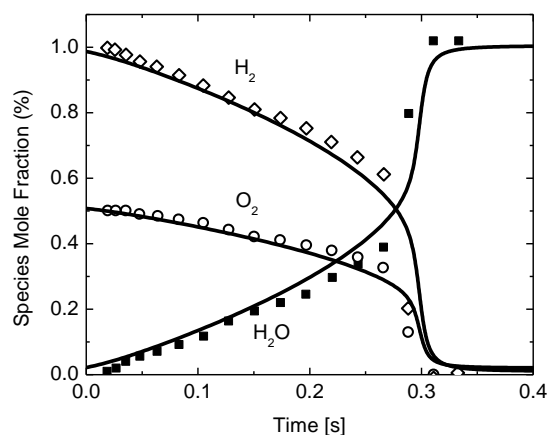

Figure S14. Species profiles from a flow reactor experiment [2]. Unburnt mixture was at 933 K, 3.4 atm and consisting of 1.01% H_2, 0.52% O_2, and N_2 balance gas. The curves are calculated with the presented mechanism by using adiabatic approximation and are shifted simultaneously by 0.35 s in time.

Figure S15. Species profiles from a flow reactor experiment [2]. Unburnt mixture was at 934 K, 6.0 atm and consisting of 1.01% H_2, 0.52% O_2, and N_2 balance gas. The curves are calculated with the presented mechanism by using adiabatic approximation and are shifted simultaneously by 0.34 s in time.
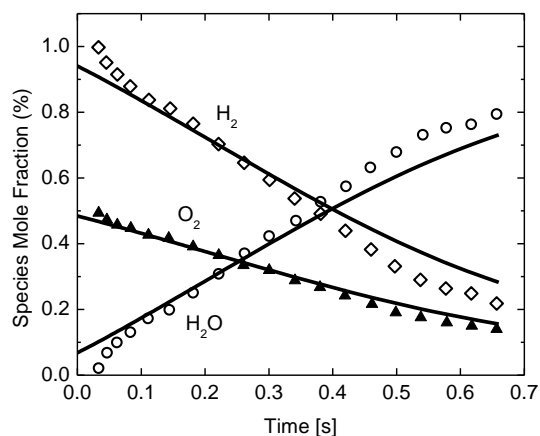

Figure S16. Species profiles from a flow reactor experiment [2]. Unburnt mixture was at 880 K, 0.32 atm and consisting of 0.5% H_2, 0.5% O_2, and N_2 balance gas. The curves are calculated with the presented mechanism by using adiabatic approx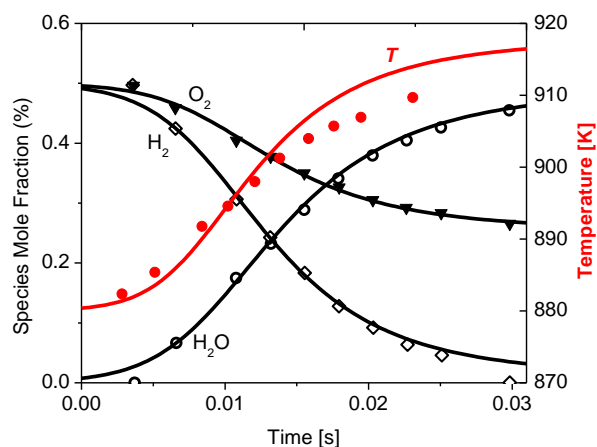imation and are shifted simultaneously by 0.069 s in time. The calculated adiabatic temperature profile is also compared with experimental values.
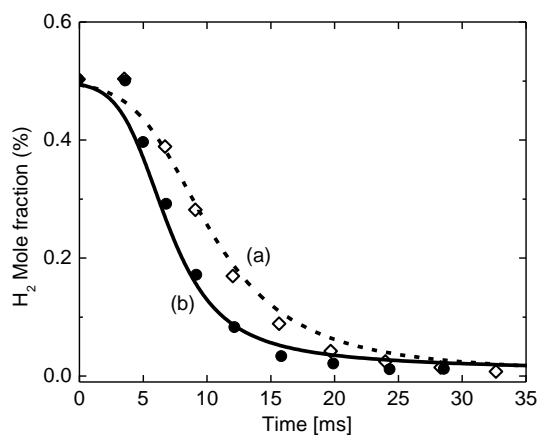
Figure S17. H_2 mole fraction profiles from a flow reactor experiment [2]. (a): 897 K, 0.60 atm, 0.50% H_2/0.34% O_2/N_2, $\phi = 0.75$, time shift =75 ms; (b) 896 K, 0.60 atm, 0.50% H_2/0.76% O_2/N_2, $\phi = 0.33$, time shift = 48 ms.
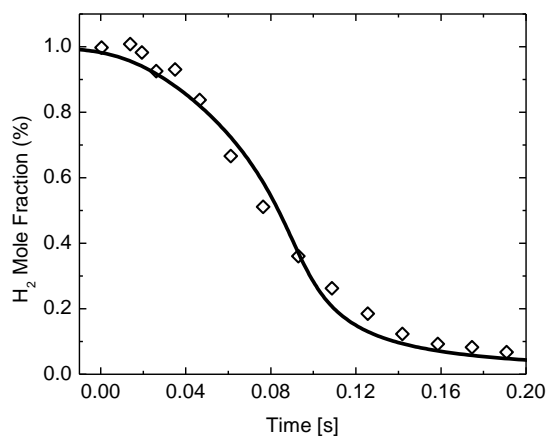

Figure S18. H_2 mole fraction profile from a flow reactor experiment [2]. Unburnt mixture was at 943 K, 2.5 atm and consisting of 1% H_2, 1.5% O_2, and N_2 balance gas. The H_2 time-history was shifted forward by 0.23 s in time.
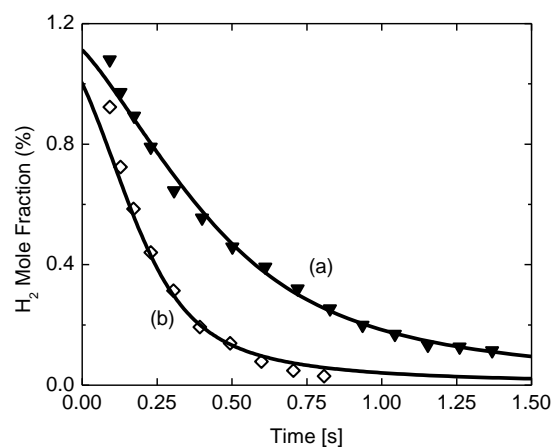
Figure S19. H_2 mole fraction profiles from a flow reactor experiment [2]. (a): 914 K, 15.7 atm, 1.18% H_2/0.61% O_2/N_2, ϕ = 1, time shift = 0.27 s; (b) 914 K, 15.7 atm, 1.18% H_2/2.21% O_2/N_2, ϕ = 0.27, time shift = 0.31 s.
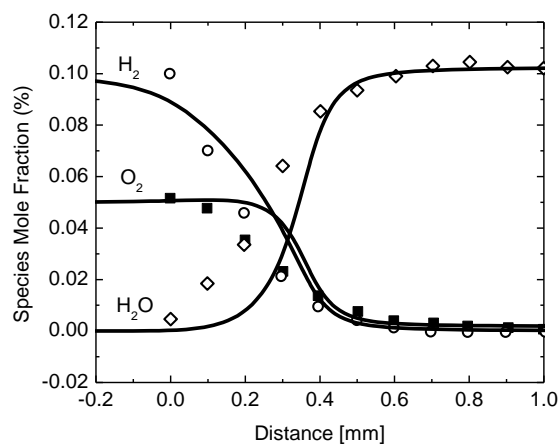

Figure S20. The structure of a burner-stabilized flame studied using a mixture of 10% H_2, 5% O_2 and balance Ar (by mole) at 10 atm and 363 K, mass flow rate: 0.135 [g cm^{-2}s^{-1}]. Experimental data are from the study by Paletskii et al. [100]; and the curves are calculated using the current mechanism.