SUPPORTING INFORMATION

Ab Initio and Transition State Theory Study of the OH + $HO_2 \rightarrow H_2O + O_2(^3\Sigma_g^-)/O_2(^1\Delta_g)$ Reactions: Yield and Role of $O_2(^1\Delta_g)$ in H_2O_2 Decomposition and in Combustion of H_2

M. Monge-Palacios, S. Mani Sarathy

The results of the flame speeds of the H_2-Air and H_2-22.18% $O_2(^3\Sigma_g^-)$ + 1.11% $O_2(^1\Delta_g)$ + 76.71% N_2 mixtures at 1 atm and 300 K are shown in Figure S1 at different equivalent ratios, ϕ, using Konnov's and our updated model.

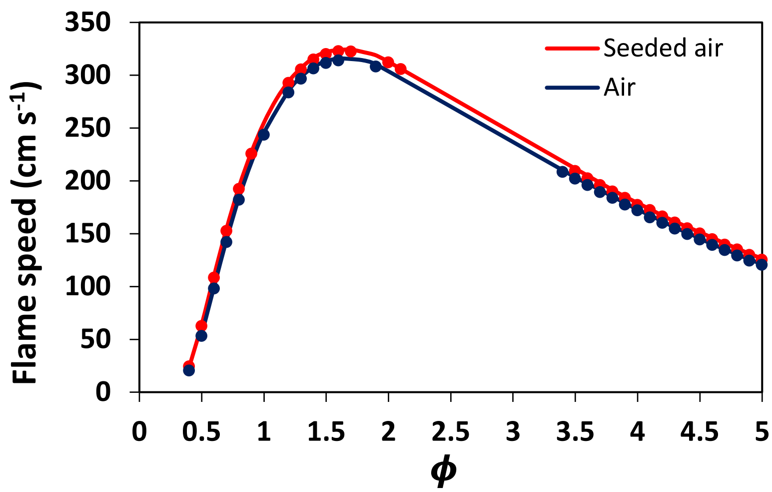

Figure S1. Flame speed of the H_2-Air (blue line) and H_2-22.18% $O_2(^3\Sigma_g^-)$ + 1.11% $O_2(^1\Delta_g)$ + 76.71% N_2 (red line) mixtures as function of equivalent ratio using Konnov's (points) and our updated model (solid line).

Both models predict similar results, with no effect of the new kinetic information for the OH + $HO_2 \rightarrow H_2O + O_2(^1\Delta_g)$ reaction. However, in mixtures seeded with O_3 small differences appear in the flame speed. These results are shown in Figure S2 for a mixture H_2-60.9% $O_2(^3\Sigma_g^-)$ + 39.1% O_3; it can be seen that our updated model predicts a slightly larger flame speed. For instance, at the equivalent ratio of 0.7 the flame speed becomes around 3.7% larger than that predicted by Konnov's model.

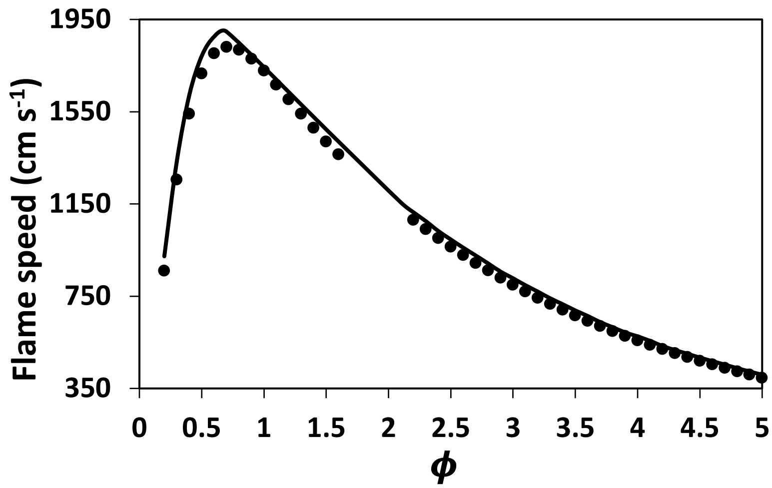

Figure S2. Flame speed of the H_2-60.9% $O_2(^3\Sigma_g^-)$ + 39.1% O_3 mixtures as function of equivalent ratio using Konnov's (points) and our updated model (solid line).

In Figure S3 the ignition delay time (based on d[OH]/dt) obtained with both models is plotted in the temperature range 900–2000 K for the mixture 0.81% H_2 + 4.03% $O_2(^3\Sigma_g^-)$ + Ar at different initial pressures. No differences were found with respect to Konnov's model predictions.

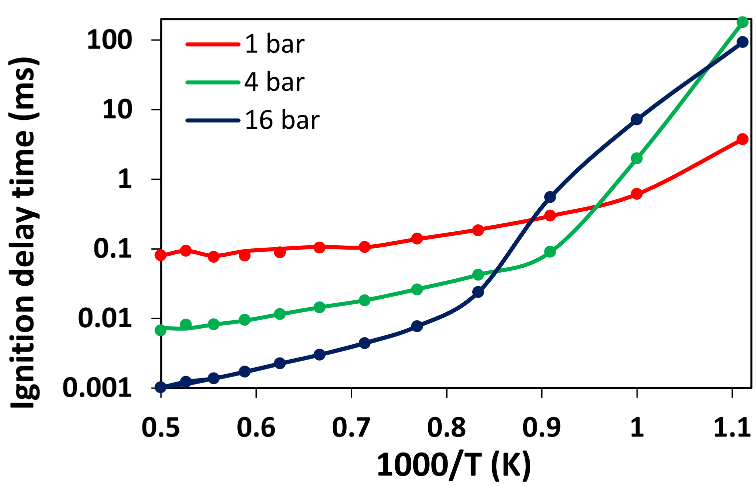

Figure S3. Ignition delay time of the 0.81% H_2 + 4.03% $O_2(^3\Sigma_g^-)$ + Ar mixture as function of temperature using Konnov's (points) and our updated model (solid line) at different pressures.