**GROUP A 109--125**

H + O2=OH + O (A-RI) -- do not have a file for

OH + H2 = H2O + H (A-R2)-- have file reaction looks bad at low temperatures

O + H2 = OH + H (A-R3)— looks good

* This reaction also doesn’t look right

|  |  |
| --- | --- |
| B1 Frequencies | 0.1 |
| B1 Energy | 2.3 |
| P2 Energy | 2.3 |
| P2 Frequencies | .045 |
| P1 Symmetry | 1e-6 |
| P1\_Frequencies\_1 | .045 |
| B1\_ImaginaryFrequency\_1 | .18 |
| P2\_SymmetryFactor\_1 | 1e-6 |
| B1\_SymmetryFactor\_1 | 1e-6 |
| P1\_Energy\_1 | 2.3 |

109 -- Z. Hong, D.F. Davidson, E.A. Barbour, R.K. Hanson. A new shock tube study of the H + O2 = OH+ O reaction rate using tunable diode laser absorption of H2O near 2.5 μm. Proceedings of the Combustion Institute 33 (2011) 309–316.

* Hong\_OH\_O\_raw\_data\_0.yaml
* Hong\_OH\_O\_raw\_data\_1.yaml

110 -- D.A. Masten, R.K. Hanson, C.T. Bowman. Shock Tube Study of the Reaction H + O2 = OH + O Using OH Laser Absorption. Journal of Physical Chemistry 94 (1990) 7119-7128.

* Should I be using the incident shock wave or the reflected shock wave?
  + Right now I am using incident shock waves
* Masten\_0.yaml – Made them from table 2 in paper, have all of them
* Masten\_11.yaml
* Masten\_26.yaml
* How much of these curves should be weighted ?
  + “The rate constant of k2 was determined by fitting the region of rapid OH evolution”

111-- A.N. Pirraglia, J.V. Michael, J.W. Sutherland, R.E. Klemm. A Flash Photolysis-Shock Tube Kinetic StudyoftheHAtomReactionwithO2:H+O2 =OH+O(962K<T<1705K) and H+O2 +Ar= HO2 + Ar (746 K < T < 987 K). *Journal of Physical Chemistry A* 93 (1989) 282-291.

* ['Pirraglia\_38.yaml'], #21
* ['Pirraglia\_59.yaml'], #22
* ['Pirraglia\_44.yaml'],#23

112 -- S.K. Wang, D.F. Davidson, R.K. Hanson. Shock Tube and Laser Absorption Study of CH2O Oxidation via Simultaneous Measurements of OH and CO. *Journal of Physical Chemistry A* 121 (2017) 8561-8568.

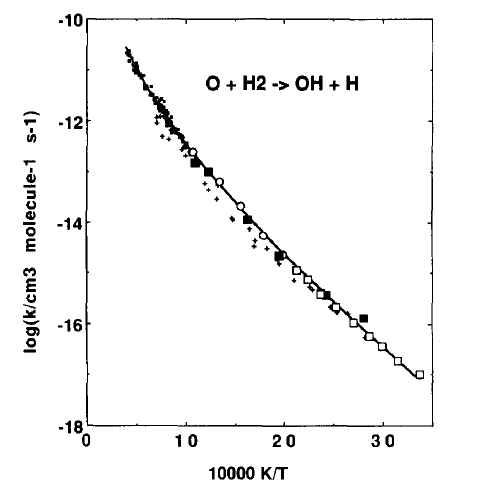
* The current study particularly focuses on the slopes of OH formation and CO depletion and the peak OH concentration
  + Weighting only OH increasing slope and CO depletion slope

From the supplemental material (should double check but looks good for now)

* ['Wang\_raw\_data\_OH\_CO\_0.yaml'],#29
* ['Wang\_raw\_data\_OH\_CO\_1.yaml'],#30
* ['Wang\_raw\_data\_OH\_CO\_2.yaml'],#31
* ['Wang\_raw\_data\_OH\_CO\_3.yaml'],#32
* ['Wang\_raw\_data\_OH\_CO\_4.yaml'],#33
* ['Wang\_raw\_data\_OH\_CO\_5.yaml'],#34
* ['Wang\_raw\_data\_OH\_CO\_6.yaml'],#35

113 -- J.V. Michael. Measurement of Thermal Rate Constants by Flash or Laser Photolysis in Shock Tubes: Oxidations of H2 and D2. *Progress in Energy and Combustion Science* 18 (1992) 327-347.

* Paper has plots of O+H2-> OH+H
* Paper has plot of H+H2O->H2+OH
* Plots are unclear because markers are all the same color and size, also axis are unclear. Markers are supposed to be small squares but it is almost impossible to tell which are which
  + Kept an excel Michael 1991 graph read rate constants excel



114 -- J.V. Michael, J.W. Sutherland. Rate Constant for the Reaction of H with H,O and OH with H, by the Flash Photolysis-Shock Tube Technique over the Temperature Range 1246-2297 K. *Journal of Physical Chemistry* 92 (1998) 3853-3857.

* Results look reasonable but not great. MSI seems to be splitting the difference should I not be weighting early data points? We previously had this dataset unweighted but unclear if it is good enough to keep?
* ['michael\_0.yaml'],
* ['michael\_9.yaml'],
* ['michael\_10.yaml'],
* ['michael\_16.yaml'],
* ['michael\_18.yaml'],
* ['michael\_19.yaml'],
* ['michael\_21.yaml'],
* ['michael\_23.yaml'],
* ['michael\_26.yaml'],
* ['michael\_28.yaml'],
* ['michael\_29.yaml'],
* ['michael\_31.yaml'],

115 -- R.C. Oldenborg, G.W. Loge, D.M. Harradine, and K.R. Winn. Kinetic Study of the OH + H2 Reaction from 800 to 1550 K. *Journal of Physical Chemistry* 96 (1992) 8426-8430.

* Table I (OH+H2 = H+H2O) (might want to double check units I think its in molecules but paper isn’t super clear)
* .693 uncertainty… what should it be ?

|  |  |
| --- | --- |
| Temperature | k 10^12 cm^3 s^-1 |
| 809 | 1.068 |
| 858 | 1.335 |
| 908 | 1.640 |
| 977 | 2.143 |
| 1011 | 2.326 |
| 1077 | 3.020 |
| 1080 | 3.055 |
| 1086 | 3.162 |
| 1111 | 3.131 |
| 1181 | 40166 |
| 1212 | 4.080 |
| 1213 | 4.249 |
| 1281 | 5.159 |
| 1282 | 5.104 |
| 1312 | 4.952 |
| 1343 | 5.767 |
| 1397 | 6.487 |
| 1413 | 6.110 |
| 1513 | 7.261 |
| 1548 | 7.875 |

116 -- L.N. Krasnoperov, J. V. Michael. Shock Tube Studies Using a Novel Multipass Absorption Cell: Rate Constant Results For OH + H2 and OH + C2H6. *Journal of Physical Chemistry A* 108 (2004) 5643-5648.

Invovles the breakdown of C4H10O2 which currently we do not have a good mechanism to accommodate. Working on it now. In the meantime using the raw rate constant data from the paper.

|  |  |
| --- | --- |
| Temperature | k |
| 11381001 |  |
| 1219 |  |
| 832 |  |
| 1037 |  |
| 11359 |  |
| 988 |  |
| 894 |  |

* Krasnoperov\_0.yaml
* Krasnoperov\_1.yaml

117-- J.V. Michael. Rate Constants for the Reaction O + D2 = OD + D by the Flash Photolysis-Shock Tube Technique over the Temperature Range 825−2487K: The H2 to D2 Isotope Effects. *Journal of Chemical Physics* 90 (1989) 189−198.

* Not using D2

118 -- J.W. Sutherland, J.V. Michael, A.N. Pirraglia, F.L. Nesbitt, R.B. Klemm. Rate Constant for the Reaction of O(3P) with H2 by the Flash Photolysis-Shock Tube and Flash Photolysis-Resonance Fluorescence Techniques; 504K ≤ T ≤ 2495K. *Proceedings of the Combustion Institute* 21 (1986) 929−941

* From Table I in paper
* Sutherland\_0.yaml and others

119 -- K.-Y. Lam, D.F. Davidson, R.K. Hanson. A Shock Tube Study of H2 + OH → H2O + H Using OH Laser Absorption. *International Journal of Chemical Kinetics* 45 (2013) 363–373.

* ['Lam\_H2O\_H\_0.yaml'],#24
* ['Lam\_H2O\_H\_1.yaml'],#25
* ['Lam\_H2O\_H\_2.yaml'],#26
* ['Lam\_H2O\_H\_3.yaml'],#27
* ['Lam\_H2O\_H\_4.yaml'],#28

120 -- H. Li, Z.C. Owens, D.F. Davidson and R.K. Hanson, "A Simple Reactive Gasdynamics Model for the Computation of Gas Temperature and Species Concentrations behind Reflected Shock Waves,” *International Journal of Chemical Kinetics* 40 (2008) 189-198.

* Variable pressure shock tube can’t do it with Cantera

121 -- J.A. Miller, M.J. Pilling, J. Troe. Unravelling combustion mechanisms through a quantitative understanding of elementary reactions. *Proceedings of the Combustion Institute* 30 (2005) 43–88.

* No easy to use raw data

122 -- J. Troe, V.G. Ushakov. Theoretical studies of the HO+O=HO2=H+O2 reaction. II. Classical trajectory calculations on an ab initio potential for temperatures between 300 and 5000 K. *Journal of Chemical Physics* 115 (2001) 3621–3628.

* No easy to use raw data

123 -- T.L. Nguyen, J.F. Stanton. Accurate ab Initio Thermal Rate Constants for Reaction of O(3P) with H2 and Isotopic Analogues. *Journal of Physical Chemistry A* 118 (2014) 4918−4928.

* NO easy to use raw data

124 -- N. Balakrishnan. Quantum calculations of the O(3P)+H2-->OH+H reaction. *Journal of Chemical Physics* 121 (2004) 6346.

* No easy to use raw data

125 -- T.L. Nguyen, J.F. Stanton, J.R. Barker. Ab Initio Reaction Rate Constants Computed Using Semiclassical Transition-State Theory: HO + H2 = H2O + H and Isotopologues. *Journal of Physical Chemistry A* 115 (2011) 5118–5126.

* No easy to use raw data