

H₂/O₂ reaction mechanism used in Donovan, M.T., Hall, D.L., Torek, P.V., Schrock, C.R., and Wooldridge, M.S., Proc. Combust. Inst. 29 (2002), in press.

Units are in cal, cm³, mol and s. Rate coefficients are expressed in the form $k = A T^b \exp(-E_a/RT)$. Thermochemical data for all species are from Kee et al. [1].

	Reaction	A	b	E _a [cal mol ⁻¹]	
1.	OH + OH = H ₂ O + O	3.57×10 ⁴	2.4	-2112.0	[2]
2.	H + O ₂ = OH + O	9.33×10 ¹³	0.0	14800.0	[3]
3.	H + OH + M = H ₂ O + M	8.34×10 ²¹	-2.0	0.0	[4]
	H ₂ O enhanced by 16.96				
4.	H + O + M = OH + M	6.20×10 ¹⁶	-0.6	0.0	[5]
	H ₂ O enhanced by 5				
5.	OH + H ₂ = H ₂ O + H	1.17×10 ⁹	1.3	3626.0	[5]
6.	H ₂ + O = OH + H	5.06×10 ⁴	2.67	6290.0	[5]
7.	O + HO ₂ = O ₂ + OH	1.40×10 ¹³	0.0	1073.0	[5]
8.	H + HO ₂ = OH + OH	1.40×10 ¹⁴	0.0	1073.0	[5]
9.	H ₂ + O ₂ = H + HO ₂	3.30×10 ¹³	0.0	53900.0	[3]
10.	OH + HO ₂ = H ₂ O + O ₂	7.50×10 ¹²	0.0	0.0	[5]
11.	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂	2.00×10 ¹²	0.0	0.0	[5]
12.	H ₂ O ₂ + OH = H ₂ O + HO ₂	1.00×10 ¹³	0.0	1800.0	[5]
13.	H ₂ O ₂ + H = H ₂ O + OH	1.00×10 ¹³	0.0	3585.0	[6]
14.	H ₂ O ₂ + H = HO ₂ + H ₂	1.60×10 ¹²	0.0	3800.0	[5]
15.	H ₂ O ₂ + O = HO ₂ + OH	2.80×10 ¹³	0.0	6405.0	[6]
16.	H ₂ O ₂ + M = OH + OH + M	1.30×10 ¹⁷	0.0	45500.0	[5]
17.	H + H + M = H ₂ + M	6.40×10 ¹⁷	-1.0	0.0	[7]
	O ₂ enhanced by 1.6, H ₂ enhanced by 0, H ₂ O enhanced by 0				
18.	H + H + H ₂ = H ₂ + H ₂	8.96×10 ¹⁶	-0.6	0.0	[7]
19.	H + H + H ₂ O = H ₂ + H ₂ O	6.00×10 ¹⁹	-1.25	0.0	[7]
20.	H ₂ + HO ₂ = H ₂ O + OH	2.00×10 ¹¹	0.0	24000.0	[8]
21.	O + O + M = O ₂ + M	1.89×10 ¹³	0.0	-1788.0	[9]
22.	H + O ₂ + M = HO ₂ + M	6.17×10 ¹⁷	-0.80	0.0	[4]
	O ₂ enhanced by 0, N ₂ enhanced by 0, H ₂ O enhanced by 0				
23.	H + O ₂ + H ₂ O = HO ₂ + H ₂ O	1.56×10 ¹⁸	-0.80	0.0	[4]
24.	H + O ₂ + O ₂ = HO ₂ + O ₂	6.70×10 ¹⁹	-1.42	0.0	[10]

References

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