

H<sub>2</sub>/O<sub>2</sub> Reaction Mechanism (unit: cm<sup>3</sup>, mol, s, kJ, K)

	Reaction	<i>A</i>	<i>n</i>	<i>E<sub>a</sub></i>
1	H + O <sub>2</sub> = O + OH	2.0 × 10 <sup>14</sup>	0.0	70.3
2	H <sub>2</sub> + O = OH + H	5.06 × 10 <sup>4</sup>	2.67	26.3
3	H <sub>2</sub> + OH = H <sub>2</sub> O + H	1.0 × 10 <sup>8</sup>	1.6	13.8
4	OH + OH = H <sub>2</sub> O + O	1.5 × 10 <sup>9</sup>	1.14	0.42
5	H + H + M = H <sub>2</sub> + M	1.8 × 10 <sup>18</sup>	-1.0	0.0
6	H + OH + M = H <sub>2</sub> O + M	2.2 × 10 <sup>14</sup>	-2.0	0.0
7	O + O + M = O <sub>2</sub> + M	2.9 × 10 <sup>17</sup>	-1.0	0.0
8	H + O <sub>2</sub> + M = HO <sub>2</sub> + M	2.3 × 10 <sup>18</sup>	-0.8	0.0
9	HO <sub>2</sub> + H = OH + OH	1.5 × 10 <sup>14</sup>	0.0	4.2
10	HO <sub>2</sub> + H = H <sub>2</sub> + O <sub>2</sub>	2.5 × 10 <sup>13</sup>	0.0	2.9
11	HO <sub>2</sub> + H = H <sub>2</sub> O + O	3.0 × 10 <sup>13</sup>	0.0	7.2
12	HO <sub>2</sub> + O = OH + O <sub>2</sub>	1.8 × 10 <sup>13</sup>	0.0	-1.7
13	HO <sub>2</sub> + OH = H <sub>2</sub> O + O <sub>2</sub>	6.0 × 10 <sup>13</sup>	0.0	0.0
14	HO <sub>2</sub> + HO <sub>2</sub> → H <sub>2</sub> O <sub>2</sub> + O <sub>2</sub>	2.5 × 10 <sup>11</sup>	0.0	-5.2
15	OH + OH + M = H <sub>2</sub> O <sub>2</sub> + M	3.25 × 10 <sup>22</sup>	-2.0	0.0
16	H <sub>2</sub> O <sub>2</sub> + H = H <sub>2</sub> + HO <sub>2</sub>	1.7 × 10 <sup>12</sup>	0.0	15.7
17	H <sub>2</sub> O <sub>2</sub> + H = H <sub>2</sub> O + OH	1.0 × 10 <sup>13</sup>	0.0	15.0
18	H <sub>2</sub> O <sub>2</sub> + O = OH + HO <sub>2</sub>	2.8 × 10 <sup>13</sup>	0.0	26.8
19	H <sub>2</sub> O <sub>2</sub> + OH = H <sub>2</sub> O + HO <sub>2</sub>	5.4 × 10 <sup>12</sup>	0.0	4.2

Efficiency factors are H<sub>2</sub>=1.0; O<sub>2</sub>=0.25; H<sub>2</sub>O=6.5

Thermodynamic database

H02	J 3/64H	10	200	000	0G	300.000	5000.000		1
	0.37866280E 01	0.27885404E-02	-0.10168708E-05	0.17183946E-09	-0.11021852E-13				2
	0.11888500E 04	0.48147611E 01	0.35094850E 01	0.11499670E-02	0.58784259E-05				3
	-0.77795519E-08	0.29607883E-11	0.13803331E 04	0.68276325E 01					4
H2	J 3/77H	2	0	0	0G	300.000	5000.000		1
	0.30667095E+01	0.57473755E-03	0.13938319E-07	-0.25483518E-10	0.29098574E-14				2
	-0.86547412E+03	-0.17798424E+01	0.33553514E+01	0.50136144E-03	-0.23006908E-06				3
	-0.47905324E-09	0.48522585E-12	-0.10191626E+04	-0.35477228E+01					4
H20	J 3/79H	20	1	0	0G	300.000	5000.000		1
	0.26110472E+01	0.31563130E-02	-0.92985438E-06	0.13331538E-09	-0.74689351E-14				2
	-0.29868167E+05	0.72091268E+01	0.41677234E+01	-0.18114970E-02	0.59471288E-05				3
	-0.48692021E-08	0.15291991E-11	-0.30289969E+05	-0.73135474E+00					4
H202	L 2/69H	20	20	00	0G	300.000	5000.000		1
	0.45731667E 01	0.43361363E-02	-0.14746888E-05	0.23489037E-09	-0.14316536E-13				2
	-0.18006961E 05	0.50113696E 00	0.33887536E 01	0.65692260E-02	-0.14850126E-06				3
	-0.46258055E-08	0.24715147E-11	-0.17663147E 05	0.67853631E 01					4
O	J 3/77O	100	000	000	0G	300.000	5000.000		R1
	0.25342961E+01	-0.12478170E-04	-0.12562724E-07	0.69029862E-11	-0.63797095E-15				2
	0.29231108E+05	0.49628591E+01	0.30309401E+01	-0.22525853E-02	0.39824540E-05				3
	-0.32604921E-08	0.10152035E-11	0.29136526E+05	0.26099342E+01					4
OH	J 6/77O	1H	10	00	0G	300.000	5000.000		R1
	0.28897814E+01	0.10005879E-02	-0.22048807E-06	0.20191288E-10	-0.39409831E-15				2
	0.38857042E+04	0.55566427E+01	0.38737300E+01	-0.13393772E-02	0.16348351E-05				3
	-0.52133639E-09	0.41826974E-13	0.35802348E+04	0.34202406E+00					4
O2	J 3/77O	20	00	00	0G	300.000	5000.000		1
	0.36122139E+01	0.74853166E-03	-0.19820647E-06	0.33749008E-10	-0.23907374E-14				2
	-0.11978151E+04	0.36703307E+01	0.37837135E+01	-0.30233634E-02	0.99492751E-05				3
	-0.98189101E-08	0.33031825E-11	-0.10638107E+04	0.36416345E+01					4
H	J 9/65H	100	000	000	0G	300.000	5000.000		R1
	0.25000000E 01	0.	0.	0.	0.				2
	0.25471627E 05	-0.46011763E 00	0.25000000E 01	0.	0.				3
	0.	0.	0.25471627E 05	-0.46011762E 00					4