## База данных процессов с участием

## колебательно-возбужденного озона

В таблице 1 представлена созданная на основе анализа данных литературы и собственных результатов база данных процессов с участием колебательновозбужденного озона. Константы скорости некоторых процессов представлены формулой Аррениуса

$$k(T) = A\left(\frac{T}{298 \text{ K}}\right)^n e^{-\frac{E_a}{RT}},$$

где А - коэффициент пропорциональности (частотный фактор),

Т – температура,

Еа – энергия активации,

R = 8.314472 × 10<sup>-3</sup> кДж/моль×К – универсальная газовая постоянная.

Размерности представленных значений констант скорости зависят от порядка реакции:

для реакций первого порядка (1/с),

второго порядка (см<sup>3</sup>/с),

третьего порядка (см<sup>6</sup>/с).

Для процессов (75) – (85) в столбце для констант скорости указан соответствующий коэффициент Эйнштейна А<sub>е</sub>.

№	Реакция	Т, К	Константа скорости k(T)	А	Еа, кДж/ моль	n	Метод	Лит.
1	$O + O_2 + CH_4 \leftrightarrow O_3(v) + CH_4$	200 - 3000	2.32×10 <sup>-27</sup>			-2.4	эксп-т	[1]
2	$O + O_2 + N_2 \leftrightarrow O_3(v) + N_2$	200 - 5000	4.7×10 <sup>-27</sup>			-2.8	теория	[13]
3	$O + O_2 + O_2 \leftrightarrow O_3(v) + O_2$	200-5000	5.1×10 <sup>-27</sup>			-2.8	теория	[2]
	$O + O_2 + O_2, N_2 \leftrightarrow O_3(000) + O_2, N_2$	500-2000	7.68×10 <sup>-35</sup> ; T=500 K	2.79×10 <sup>-35</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_3(001) + O_2, N_2$	500-2000	5.38×10 <sup>-35</sup> ; T=500 K	2.32×10 <sup>-35</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_3(002) + O_2, N_2$	500-2000	5.09×10 <sup>-35</sup> ; T=500 K	1.85×10 <sup>-35</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_3(003) + O_2, N_2$	500-2000	3.91×10 <sup>-35</sup> ; T=500 K	1.42×10 <sup>-35</sup>	4240		эксп-т	[3]
4	$\leftrightarrow O_{3}(004) + O_{2}, N_{2}$	500-2000	2.91×10 <sup>-35</sup> ; T=500 K	1.06×10 <sup>-35</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_3(005) + O_2, N_2$	500-2000	2.08×10 <sup>-35</sup> ; T=500 K	7.59×10 <sup>-36</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_3(006) + O_2, N_2$	500-2000	1.3×10 <sup>-35</sup> ; T=500 K	4.73×10 <sup>-36</sup>	4240		эксп-т	[3]
	$\leftrightarrow O_{3}(007) + O_{2}, N_{2}$	500-2000	6.96×10 <sup>-36</sup> ; T=500 K	2.53×10 <sup>-36</sup>	4240		эксп-т	[3]
	$\leftrightarrow \mathrm{O}_3(008) + \mathrm{O}_2, \mathrm{N}_2$	500-2000	2.42×10 <sup>-37</sup> ; T=500 K	8.80×10 <sup>-37</sup>	4240		эксп-т	[3]
5	$O_3(008) + O \rightarrow O_2 + O_2$	500-2000	1×10 <sup>-11</sup>				эксп-т	[3]
6	$O_3(007) + O \rightarrow O_2 + O_2$	500-2000	$1 \times 10^{-11}$				эксп-т	[3]
7	$O_3(006) + O \rightarrow O_2 + O_2$	500-2000	$1 \times 10^{-11}$				эксп-т	[3]
8	$O_3(005) + O \rightarrow O_2 + O_2$	500-2000	$1 \times 10^{-11}$				эксп-т	[3]
9	$O_3(004) + O \rightarrow O_2 + O_2$	500-2000	$1 \times 10^{-11}$				эксп-т	[3]
10	$O_3(003) + O \rightarrow O_2 + O_2$	500-2000	$1 \times 10^{-11}$				эксп-т	[3]
11	$O_3(002) + O \rightarrow O_2 + O_2$	500-2000	1×10 <sup>-11</sup>				эксп-т	[3]
12	$O_3(001) + O \rightarrow O_2 + O_2$	500-2000	1×10 <sup>-11</sup>				эксп-т	[3]
	$O_3(000) + hv \rightarrow O_3(001)$	500-2000	$6.4 \times 10^{-3}$				эксп-т	[3]
13	$\rightarrow$ O <sub>3</sub> (010)	500-2000	6.7×10 <sup>-3</sup>				эксп-т	[3]
	$\rightarrow$ O <sub>3</sub> (100)	500-2000	$1.2 \times 10^{-4}$				эксп-т	[3]
	$\rightarrow$ O <sub>3</sub> (101)	500-2000	4.2×10 <sup>-5</sup>				эксп-т	[3]

## Таблица 1 – База данных процессов с участием колебательно-возбужденного озона

14	$O_3(000) + O_2, N_2 \rightarrow O_3(001) + O_2, N_2$	500-2000	1×10 <sup>-15</sup> ; T=500 K	$2.0 \times 10^{-14}$	-12471	эксп-т	[3]
15	$O_3(008) + O_2, N_2 \rightarrow O_3(007) + O_2, N_2$	500-2000	$(2.3 \times 10^{-14}) T^{1/2}$			эксп-т	[3]
16	$O_3(007) + O_2, N_2 \rightarrow O_3(006) + O_2, N_2$	500-2000	$(2.0 \times 10^{-14}) T^{1/2}$			эксп-т	[3]
17	$O_3(006) + O_2, N_2 \rightarrow O_3(005) + O_2, N_2$	500-2000	$(1.7 \times 10^{-14}) T^{1/2}$			эксп-т	[3]
18	$O_3(005) + O_2, N_2 \rightarrow O_3(004) + O_2, N_2$	500-2000	$(1.4 \times 10^{-14}) T^{1/2}$			эксп-т	[3]
19	$O_3(004) + O_2, N_2 \rightarrow O_3(003) + O_2, N_2$	500-2000	$(1.2 \times 10^{-14}) T^{1/2}$			эксп-т	[3]
20	$O_3(003) + O_2, N_2 \rightarrow O_3(002) + O_2, N_2$	500-2000	$(8.7 \times 10^{-15})$ T <sup>1/2</sup>			эксп-т	[3]
21	$O_3(002) + O_2, N_2 \rightarrow O_3(001) + O_2, N_2$	500-2000	$(5.8 \times 10^{-15}) T^{1/2}$			эксп-т	[3]
22	$O_3(001) + O_2, N_2 \rightarrow O_3(000) + O_2, N_2$	500-2000	$(2.9 \times 10^{-15}) T^{1/2}$			эксп-т	[3]
23	$O_3(000) + O \rightarrow O_3(001) + O$	500-2000	5×10 <sup>-13</sup> ; T=500 K	$1.0 \times 10^{-11}$	-12471	эксп-т	[3]
24	$O_3(000) + O_2, N_2, O \rightarrow O_3(010) + O_2, N_2, O$	500-2000	3.9×10 <sup>-15</sup> ; T=500 K	3.0×10 <sup>-14</sup>	-8380	эксп-т	[3]
25	$O_3(001) + O_2, N_2, O \rightarrow O_3(100) + O_2, N_2, O$	500-2000	1×10 <sup>-11</sup>			эксп-т	[3]
26	$O_3(100) + O_2, N_2, O \rightarrow O_3(001) + O_2, N_2, O$	500-2000	8.3×10 <sup>-12</sup> ; T=500 K	1×10 <sup>-11</sup>	-731	эксп-т	[3]
27	$O_3(002) + O_2, N_2, O \rightarrow O_3(101) + O_2, N_2, O$	500-2000	1×10 <sup>-11</sup>			эксп-т	[3]
28	$O_3(101) + O_2, N_2, O \rightarrow O_3(002) + O_2, N_2, O$	500-2000	1×10 <sup>-11</sup>			эксп-т	[3]
29	$O_3(001) + O_2, N_2, O \rightarrow O_3(010) + O_2, N_2, O$	500-2000	$5 \times 10^{-14}$			эксп-т	[3]
30	$O_3(100) + O_2, N_2, O \rightarrow O_3(010) + O_2, N_2, O$	500-2000	5×10 <sup>-14</sup>			эксп-т	[3]
31	$O_3(010) + O_2, N_2, O \rightarrow O_3(000) + O_2, N_2, O$	500-2000	3×10 <sup>-14</sup>			эксп-т	[3]
32	$O_3(010) + O_2, N_2, O \rightarrow O_3(100) + O_2, N_2, O$	500-2000	$1.58 \times 10^{-14}$ ; T=500 K	5×10 <sup>-14</sup>	-4813	эксп-т	[3]
33	$O_3(010) + O_2, N_2, O \rightarrow O_3(001) + O_2, N_2, O$	500-2000	1.8×10 <sup>-14</sup> ; T=500 K	5×10 <sup>-14</sup>	-4081	эксп-т	[3]
34	$O(^{3}P) + O_{2}(X^{3}\Sigma) + O_{2}(X^{3}\Sigma) \rightarrow O_{3}(\upsilon) + O_{2}(X^{3}\Sigma)$	298	6.0×10 <sup>-34</sup> (T/300) <sup>-2.6</sup>			эксп-т	[4]
35	$O(^{3}P) + O_{2}(X^{3}\Sigma) + Ar \rightarrow O_{3}(\upsilon) + Ar$	298	$0.63 \times (6.0 \times 10^{-34} (T/300)^{-2.6})$			эксп-т	[5]
36	$O(^{3}P) + O_{2}(X^{3}\Sigma) + He \rightarrow O_{3}(\upsilon) + He$	298	5.1×10 <sup>-27</sup> T <sup>-2.8</sup>			эксп-т	[6]
37	$O(^{3}P) + O_{2}(X^{3}\Sigma) + N_{2} \rightarrow O_{3}(\upsilon) + N_{2}$	298	5.6×10 <sup>-34</sup> (T/300) <sup>-2.6</sup>			эксп-т	[7]
38	$O(^{3}P) + O_{2}(X^{3}\Sigma) + CO_{2} \rightarrow O_{3}(\upsilon) + CO_{2}$	298	1.5×10 <sup>-33</sup>			эксп-т	[8]
39	$O_3(100,001) + O_2(X^3\Sigma) \rightarrow O_3(010) + O_2(X^3\Sigma)$	298	$1.2 \times 10^{-13} T^{0.5} exp(-26.8/T^{1/3})$			эксп-т	[9]
40	$\Omega_{2}(100,001) + \Lambda r \longrightarrow \Omega_{2}(010) + \Lambda r$	298	5.9×10 <sup>-15</sup>			эксп-т	[10]
40	$O_3(100,001) + AI \rightarrow O_3(010) + AI$	298	5.6×10 <sup>-15</sup>			эксп-т	[11]
41	$O_3(010) + Ar \rightarrow O_3(000) + Ar$	298	1×10 <sup>-14</sup>			эксп-т	[10]
42	$O_2(y=1) + \Lambda r \rightarrow O_2(000) + \Lambda r$	298	7.4×10 <sup>-15</sup>			эксп-т	[11]
42	$0_{3}(0-1) + A_{1} \rightarrow 0_{3}(000) + A_{1}$	298	7.3×10 <sup>-15</sup>			эксп-т	[12]

43	$O_3(\upsilon \ge 2) + Ar \rightarrow O_3 + Ar$	298	$1 \times 10^{-14}$				эксп-т	[10]
44	$O_3(100,001) + CO_2 \rightarrow O_3(010) + CO_2$	298	2×10 <sup>-13</sup>				эксп-т	[13]
45	$O_3(010) + CO_2 \rightarrow O_3(000) + CO_2$	298	1×10 <sup>-13</sup>				эксп-т	[13]
46	$O_3(\upsilon \ge 2) + CO_2 \rightarrow O_3 + CO_2$	298	$2 \times 10^{-13}$				эксп-т	[14]
47	$O_3(\upsilon=1) + CO_2 \rightarrow O_3(000) + CO_2$	298	$1.6 \times 10^{-13}$				эксп-т	[12]
48	$O_3(000) + CO_2 (\upsilon_3=1) \rightarrow O_3 (100,001) + CO_2$	298	7.6×10 <sup>-13</sup>				эксп-т	[15]
49	$O_3(010) + He \rightarrow O_3(000) + He$	298	1×10 <sup>-13</sup>					[10]
50	$O_3(v \ge 2) + He \rightarrow O_3 + He$	298	1×10 <sup>-13</sup>				эксп-т	[10]
51	$O_3(v=1) + He \rightarrow O_3(000) + He$	298	6×10 <sup>-14</sup>				эксп-т	[12]
52	$O_3(010) + N_2 \rightarrow O_3(000) + N_2$	298	$59 \times 10^{-13} T^{0.5} exp(-53.8/T^{1/3})$				эксп-т	[10]
53	$O_3(\upsilon \ge 2) + N_2 \rightarrow O_3 + N_2$	298	$0,5 \times 10^{-13} T^{0,5} exp(-22,8/T^{1/3})$				эксп-т	[16]
54	$O_3(v) + N_2 \leftrightarrow O_3 + N_2$	200-500	4.7×10 <sup>-18</sup>			1.53	эксп-т	[9]
55	$O_3(v=1) + N_2 \rightarrow O_3(000) + N_2$	298	$1.94 \times 10^{-14}$				эксп-т	[12]
56	$O_3(100,001) + O(^{3}P) \rightarrow O_3(000) + O(^{3}P)$	298	8×10 <sup>-12</sup>				эксп-т	[17]
57	$O_3(010) + O({}^{3}P) \rightarrow O_3(000) + O({}^{3}P)$	298	8×10 <sup>-12</sup>				эксп-т	[17]
58	$O_2(a^1\Delta) + O_3(000) \rightarrow 2O_2(X^3\Sigma) + O(^3P)$	298	1.56×10 <sup>-13</sup> ; T=500 K	5.2×10 <sup>-11</sup>	-23611		эксп-т	[18]
59	$O_2(a^1\Delta) + O_3(010) \rightarrow 2O_2(X^3\Sigma) + O(^3P)$	298	$5.2 \times 10^{-11} \exp(-(2840 - E^{1,0})/T)$				эксп-т	[18]
60	$O_3(v) + O_2(a^1\Delta) \leftrightarrow O_2 + O_2 + O_2$	200 - 5000	4.1×10 <sup>-11</sup>				эксп-т	[19]
61	$O_3(000) + O \rightarrow O_3(001) + O$	298	5×10 <sup>-13</sup> ; T=500 K	$1.0 \times 10^{-11}$	-12471		эксп-т	[3]
62	$O_3(\upsilon_3=1\div8) + O \rightarrow O_2 + O_2$	298	$1.0 \times 10^{-11}$				эксп-т	[3]
63	$O_3(v) + O \leftrightarrow O_3 + O$	200 - 5000	3×10 <sup>-12</sup>				эксп-т	[19]
64	$O_3(010) + O \rightarrow O_3(000) + O$	298	3×10 <sup>-12</sup>				эксп-т	[20]
65	$O_3(100,001) + O \rightarrow O_3(010) + O(100,001)$	298	9×10 <sup>-12</sup>				эксп-т	[20]
66	$O_3(v) + O \leftrightarrow O_2 + O_2$	200-5000	1.2×10 <sup>-21</sup>				эксп-т	[19]
67	$O_3(\upsilon \ge 2) + O_2 \rightarrow O_3 + O_2$	298	$0,5 \times 10^{-13} T^{0,5} exp(-22,8/T^{1/3})$				эксп-т	[16]
68	$O_3(v=1) + O_2 \rightarrow O_3 + O_2$	298	$3 \times 10^{-15}$				эксп-т	[21]
69	$O_3(v) + O_2 \leftrightarrow O_3 + O_2$	200-5000	4.8×10 <sup>-18</sup>			1.53	эксп-т	[9]
70	$O_2(a) + O_3(\nu \ge 2) \rightarrow 2O_2(X) + O(_3P)$	298	$(4,1\times1,1)\times10^{-11}$				эксп-т	[22]
71	$O_2(a) + O_3(v=1) \rightarrow O + O_2 + O_2$	298	$2.08 \times 10^{-11}$ ; T=500 K	$26 \times 10^{-11}$	-10700		эксп-т	[23]
72	$O_3(v) + CO \rightarrow O_3 + CO$	298	$(1,5\pm0,2)\times10^{-13}$				эксп-т	[24]

73	$O_3(\upsilon \ge 2) + O(^3P) \rightarrow 2O_2(X)$	298	1.22×10 <sup>-11</sup>		эксп-т	[25]
74	$O_3(\upsilon \ge 2) + O(^3P) \rightarrow O_3 + O(_3P)$	298	2.9×10 <sup>-12</sup>		эксп-т	[25]
75	$O_3(008) \to O_3(007) + hv$	298	A <sub>e</sub> = 52.1		эксп-т	[3]
76	$O_3(007) \to O_3(006) + hv$	298	A <sub>e</sub> = 49.6		эксп-т	[3]
77	$O_3(006) \rightarrow O_3(005) + hv$	298	$A_{e} = 45.9$		эксп-т	[3]
78	$O_3(005) \to O_3(004) + hv$	298	$A_{e} = 41.4$		эксп-т	[3]
79	$O_3(004) \to O_3(003) + hv$	298	$A_{e}=35.8$		эксп-т	[3]
80	$O_3(003) \rightarrow O_3(002) + hv$	298	$A_{e}=28.9$		эксп-т	[3]
81	$O_3(002) \rightarrow O_3(001) + hv$	298	$A_{e}=20.7$		эксп-т	[3]
82	$O_3(001) \rightarrow O_3(000) + hv$	298	$A_{e}=11.2$		эксп-т	[3]
83	$O_3(101) \rightarrow O_3(000) + hv$	298	$A_{e} = 4.1$		эксп-т	[3]
84	$O_3(100) \rightarrow O_3(000) + hv$	298	$A_{e} = 0.5$		эксп-т	[3]
85	$O_3(010) \rightarrow O_3(000) + hv$	298	$A_{e}=0.25$		эксп-т	[3]
86	$O_3(100,001) + O_3 \rightarrow O_3(v=2) + O_3$	298	$1.7 \times 10^{-13}$		эксп-т	[11]
87	$O_3(010) + O_3 \rightarrow O_3(000) + O_3$	298	$8.8 \times 10^{-14}$		эксп-т	[11]
88	$O_3(100,001) + O_2 \rightarrow O_3(010) + O_2$	298	$5.2 \times 10^{-14}$		эксп-т	[26]
	$O_3(010) + O_2 \rightarrow O_3(000) + O_2$	298	3×10 <sup>-14</sup>		эксп-т	[26]
89		298	$2.27 \times 10^{-14}$		эксп-т	[27]
		298	$2.0 \times 10^{-14}$		эксп-т	[20]
00	$O_3(100,001) + O_2 \rightarrow O_3(010) + O_2$	298	$9.4 \times 10^{-15}$		эксп-т	[27]
90		298	$3.7 \times 10^{-14}$		эксп-т	[20]
91	$O_3(v=1) + O_2 \rightarrow O_3(000) + O_2$	298	$1.3 \times 10^{-14}$		эксп-т	[12]
92	$O_3(v=1) + H_2 \rightarrow O_3(000) + H_2$	298	$1.18 \times 10^{-12}$		эксп-т	[12]
93	$O_3(v=1) + D_2 \rightarrow O_3(000) + D_2$	298	$1.3 \times 10^{-13}$		эксп-т	[28]
94	$O_3(v=1) + CH_4 \rightarrow O_3(000) + CH_4$	298	4.8×10 <sup>-13</sup>		эксп-т	[12]
95	$O_3(\upsilon=1) + SO_2 \rightarrow O_3(000) + SO_2$	298	2.35×10 <sup>-13</sup>		эксп-т	[12]
96	$O_3(v=1) + SF_6 \rightarrow O_3(000) + SF_6$	298	1.6×10 <sup>-12</sup>		эксп-т	[12]
97	$O_3(\upsilon=1) + SiF_4 \rightarrow O_3(000) + SiF_4$	298	3.8×10 <sup>-11</sup>		эксп-т	[15]
98	$O_3(\upsilon=1) + \overline{H_2O \rightarrow O_3(000) + H_2O}$	298	3.5×10 <sup>-12</sup>		эксп-т	[12]
99	$O_3(100,001) + NO \rightarrow O_3(010) + NO$	350	4.8×10 <sup>-13</sup>		эксп-т	[29]

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