RECOMMENDED RATE CONSTANTS OF CHEMICAL REACTIONS IN AN H$_2$-O$_2$ GAS MIXTURE WITH ELECTRONICALLY EXCITED SPECIES O$_2$($^1\Delta$), O(^{1}D), OH($^2\Sigma$) INVOLVED

L.B. Ibraguimova, G.D. Smekhov, O.P. Shatalov

Institute of Mechanics of Lomonosov Moscow State University

Moscow, 2003

DATABASE OF RATE CONSTANTS OF CHEMICAL REACTIONS IN AN H_2-O_2 GAS MIXTURE WITH ELECTRONICALLY EXCITED SPECIES $O_2(^1\Delta)$, $O(^1D)$, $OH(^2\Sigma)$ INVOLVED

Preface

The database of recommended rate constants of chemical reactions in an H_2-O_2 gas mixture with electronically excited species $O_2(^1\Delta)$, $O(^1D)$, $OH(^2\Sigma)$ involved is presented. The chemical model includes dissociation, recombination, exchange and quenching reactions. The rate constants proposed are recommended for using for the temperature range $T = 500$–2500 K in combustion problems. Both original experimental studies and well known reviews are used.

First of all, our recommendations are based on well-known reviews of D.L. Baulch et al. [1−5], W. Tsang and R.F. Hampson [6], J. Warnatz [7], E.P. Dougherty and H. Rabitz [8], etc [9]. In a review of A.M. Starik and N.S. Titova [10] the data on reactions with electronically excited species involved were given. As a rule, these data are absent in other publications. The data on certain specific reactions including those with species excited were obtained by O.V. Skrebkov and S.P. Karkach. Those data were in part published [11−13] and in part communicated privately [14].

In our work we have used data collected in a NIST computer database (the version 2Q98, 1998 г.) [15]. This database contains the information on reviews and original experimental and theoretical, studied within a long time period.

The methods used can be divided into following groups.

1. Statistical data processing if the number of studies available made it possible. It could be performed in the NIST package [15] itself, which offers this service for the data contained in it. It could also be the statistical data processing in an "Expert" package (Institute of Mechanics). The procedure of making recommendations in the "Expert" code was described in [16]. The rate constant value obtained in the calculation was used as an original recommendation.

2. If the data presented in reviews were given for different temperature ranges, they were processed statistically in the "Expert" package. The results of this processing are recommended for the entire temperature range.

3. If the available data are widely scattered, we recommend the rate constant presented in a review of most authoritative authors or the value obtained most recently under condition that a sufficiently broad range of studies was used.

4. If the data were presented only by a single author and it is difficult to estimate the reliability of a rate constant, the reaction is included in the database within the category "Information Data" (ID).

5. The theoretical estimates of rate constants are included in the database only if other data are absent as, for example, in the case of rate estimates presented in [12, 13]. These data are also included within the "ID" category.

6. In several cases the available data on rate constants contradict to each other so that it is impossible to obtain a recommended value. Then we give no recommendation and present the corresponding publication in our commentary.

A rate constant is included in the category "Recommended Data" (RD) if there are enough data on the corresponding reaction, to perform the statistical processing and to estimate the uncertainty of the rate constant recommended using the "Expert" package [16]. The data were included in the same category if the reliable recommendation was obtained in another publication.

In the comments only category "ID" is given. If the category is not mentioned we assume by default that this is "RD".

The arguments used in developing the recommendations are given in our commentary. The recommended reaction rate constant values are given in Tables 1−5. In the tables the following notation is used: M is the collisional partner in dissociation, recombination and excited states quenching reactions, k is the recommended reaction rate constant value, $\Delta\lg k$ is the total error of the recommended rate constant. Values k and $\Delta\lg k$ determine an interval of true values of rate constants for the recommended temperature range ΔT on which all the data selected for processing are overlapped.

The recommended rate constant value is presented in the Table in the form of the generalized Arrhenius's relation:

$$k = AT^n \exp\left(-E/T\right).$$

The rate constants of dissociation / recombination of molecules are presented only in the low pressure limit. With the dimension is cm^3/mol/s for dissociation and exchange reactions, and cm^6/mol^2/s for recombination.

In the database, in certain cases the data for both the exothermic and endothermic direction of the process are presented. However, the relation $k(-)/k(+) = K_p$ (where $k(+)$ and $k(-)$ are the rate constants for the exothermic and endothermic direction, respectively) does not always hold. The reason most often is a wide scattering of the data or an unreliability of the experimental information. Therefore, we recommend to use the rate constant values for direct or reverse reactions on the temperature range for which the data are reliable and to determine the rate constant of the reverse reaction from the equilibrium constant.

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Table 1. Reactions of dissociation

Reaction	ΔT, 10^3 K	M	k, cm^3/mol/s	Δlg k	Note
H$_2$+M = 2H+M	1–8	H$_2$	$3.46\times10^{14}\cdot\exp(-48350/T)$	0.24	1
	1–8	O$_2$	$3.46\times10^{14}\cdot\exp(-48350/T)$	0.5	1
	1–8	Ar, N$_2$	$2.23\times10^{14}\cdot\exp(-48350/T)$	0.2	1
	0.6–2	H$_2$O	$8.48\times10^{19}\cdot T^{-1.1}\cdot\exp(-52530/T)$	0.7	1
O$_2$+M = 2O+M	2–4.1	Ar	$1.5\times10^{18}\cdot T^{-0.99}\cdot\exp(-59380/T)$	0.17	2
	2–5	O$_2$	$9.8\times10^{24}\cdot T^{-2.5}\cdot\exp(-59380/T)$	0.3	2
	2–5	O	$3.5\times10^{25}\cdot T^{-2.5}\cdot\exp(-59380/T)$	0.4	2
	2–5	O$_3$, H$_2$O	$1.2\times10^{19}\cdot T^{-1}\cdot\exp(-59380/T)$	1	2
O$_2$*+M = 2O+M	1–3	*)	$2.6\times10^{18}\cdot\exp(-48188/T)$	–	95
O$_3$+M = O$_2$+O+M	0.2–3	Ar	$2.48\times10^{14}\cdot\exp(-11430/T)$	0.1	3
	0.3–3	O$_2$	$1.54\times10^{14}\cdot\exp(-11600/T)$	–	3
	0.2-3	O	$2.48\times10^{15}\cdot\exp(-11430/T)$	–	3
	0.3–3	O$_3$	$4.4\times10^{14}\cdot\exp(-11600/T)$	0.2	3
	0.4–2.5	N$_2$	$4.0\times10^{14}\cdot\exp(-11400/T)$	0.6	3
O$_3$+M = O$_2$*+O+M	0.3–3	*)	$1.32\times10^{14}\cdot\exp(-11400/T)$	–	65
OH+M = O+H+M	0.3–2.5	Ar,N$_2$,O$_2$	$2.41\times10^{15}\cdot\exp(-50000/T)$	0.7	4
H$_2$O+M = H+OH+M	2–6	N$_2$	$3.5\times10^{15}\cdot\exp(-52920/T)$	0.5	4
	0.3–2.5	Ar	$4\times10^{23}\cdot T^{-2.2}\cdot\exp(-59000/T)$	0.6	4
	2–5	H$_2$O	$1.6\times10^{17}\cdot\exp(-57491/T)$	0.3	4
	2–6	O$_2$	$3.5\times10^{15}\cdot\exp(-52920/T)$	0.5	4
HO$_2$+M = H+O$_2$+M	0.5–3	N$_2$	$2.8\times10^{15}\cdot\exp(-23000/T)$	0.2	6
	0.5–3	Ar	$2.1\times10^{15}\cdot\exp(-23000/T)$	0.2	6
	0.5–3	O$_2$	$2.8\times10^{15}\cdot\exp(-23000/T)$	0.3	6
HO$_2$+M = O$_2$*+H+M	0.5–3	*)	$6.93\times10^{14}\cdot\exp(-23000/T)$	–	7
H$_2$O$_2$+M = 2OH+M	0.95–1.5	Ar	$6.0\times10^{16}\cdot\exp(-22900/T)$	0.3	8
	0.5–2.5	N$_2$	$1.2\times10^{17}\cdot\exp(-22900/T)$	0.3	8
	0.77–0.85	H$_2$	$1.33\times10^{18}\cdot\exp(-24530/T)$	–	8
	0.5–0.95	H$_2$O$_2$	$2.51\times10^{18}\cdot\exp(-24154/T)$	–	8

*) Collisional partner M is unidentified

Table 2. Reactions of recombination

Reaction	ΔT, 10^3 K	M	k, cm^6/mol^2/s	Δlg k	Note
$HO_2+HO_2+M=H_2O_2+O_2+M$	0.3	O_2	1.6×10^{16}	0.15	9
	0.23–0.42	N_2	$1.6\times10^{14}\cdot\exp(900/T)$	0.2	9
$2H+M = H_2+M$	0.5–2.5	Ar	$6.48\times10^{17}\cdot T^{-1}$	0.5	10
	0.3–5	H_2	$9.72\times10^{16}\cdot T^{-0.6}$	0.5	10
	0.3–2	H_2O	$1.0\times10^{19}\cdot T^{-1}$	0.7	10
	0.3–5	H	3.2×10^{15}	0.5	10
$2O+M = O_2+M$	0.3–4	Ar	$1.89\times10^{13}\cdot\exp(900/T)$	0.11	11
	0.5–4	O_2	$1.5\times10^{16}\cdot T^{-0.41}$	0.23	11
	0.3–2.5	N_2	$6.0\times10^{13}\cdot\exp(900/T)$	0.6	11
	0.3–4	O	$5.34\times10^{16}\cdot T^{-0.41}$	0.2	11
	0.3–4	O_3	$1.3\times10^{14}\cdot\exp(900/T)$	0.8	11
$O_2+O+M = O_3+M$	0.2–2.5	Ar	$4.3\times10^{12}\cdot\exp(1050/T)$	0.6	12
	0.2–3	O_2	$3.26\times10^{19}\cdot T^{-2.06}$	0.6	12
	0.2–3	N_2	$1.6\times10^{14}\cdot T^{-0.39}\cdot\exp(700/T)$	0.7	12
	0.22–3	O	$2.28\times10^{15}\cdot T^{-0.5}\cdot\exp(700/T)$	0.3	12
	0.22–3	O_3	$1.67\times10^{15}\cdot T^{-0.51}\cdot\exp(700/T)$	0.36	12
$O_2^*+O+M = O_3+M$	0.25–3	*)	$6.9\times10^{12}\cdot\exp(1050/T)$	–	13
$O+H+M = OH+M$	0.3–2.5	*)	$4.71\times10^{18}\cdot T^{-1}$	0.7	14
$O+H+M = OH^*+M$	0.5–3	H_2,O_2	$3.0\times10^{18}\cdot T^{-1}$	1	15
	0.5-3	Ar	$3.0\times10^{18}\cdot T^{-1}$	1	15
	0.5–3	OH	$1.49\times10^{19}\cdot T^{-1}$	1	15
$O^*+H+M = OH^*+M$	0.5–3	H_2,O_2	$4.77\times10^{18}\cdot T^{-1}$	–	16
	0.5–3	Ar	$1.49\times10^{18}\cdot T^{-1}$	–	16

	0.3–3	N_2	$2.2\times10^{22}\cdot T^{-2}$	0.5	17
	0.3–3	Ar	$8.3\times10^{21}\cdot T^{-2}$	0.3	17
H+OH+M = H$_2$O+M	0.3–3	H_2O	$1.4\times10^{23}\cdot T^{-2}$	0.5	17
	1.74–1.86	OH	8.34×10^{15}	–	17
	0.5–3	H_2	$2.0\times10^{20}\cdot T^{-1}$	–	17
	0.5–3	O_2	$2.7\times10^{18}\cdot T^{-1}$	0.7	18
	0.3–4.1	Ar	$6.1\times10^{17}\cdot T^{-0.8}$	0.5	18
H+O$_2$+M = HO$_2$+M	0.3–2	H_2	$2.09\times10^{18}\cdot T^{-0.8}$	0.5	18
	0.3–2	H_2O	$1.56\times10^{18}\cdot T^{-0.8}$	0.5	18
	0.3–2.5	N_2	$4.4\times10^{18}\cdot T^{-1}$	0.33	18
H+O$_2^*$+M = HO$_2$+M	0.25–3	*)	$1.5\times10^{15}\cdot\exp(500/T)$	–	19
	0.25–1.4	N_2	$2.2\times10^{19}\cdot T^{-0.76}$	0.4	20
OH+OH+M = H$_2$O$_2$+M	0.3–3	Ar	$6.33\times10^{23}\cdot T^{-2.53}\cdot\exp(-42/T)$	–	20
	0.3–0.4	H_2O	1.44×10^{18}	0.4	20
OH+O+M = HO$_2$+M	0.3–2.5	Ar, N$_2$	8.0×10^{16}	2.0	96

*) Collisional partner M is unidentified

Table 3. Exchange Reactions

Reaction	ΔT, 10^3 K	k, cm^3/mol/s	Δlg k	Note
$H_2+O = OH+H$	0.3–4.1	$5.1\times10^4 \cdot T^{2.67} \cdot \exp(-3160/T)$	0.5–2.	21
$H_2+O_2 = O+H_2O$	1–2.5	$3.0\times10^{13} \cdot \exp(-35000/T)$	–	22
$H_2+O_2 = H+HO_2$	0.3–4.1	$1.94\times10^{14} \cdot \exp(-29770/T)$	2.5	23
$H_2+O_2 = OH+OH$	0.76–2.5	$4.47\times10^{11} \cdot \exp(-17338/T)$	0.5	24
$H_2+2O_2 = 2HO_2$	0.5–3	$6.0\times10^{11} \cdot \exp(-4170/T)$	–	25
$H_2+O_3 = HO_2+OH$		No recommendation		26
$H_2+OH = H+H_2O$	0.2–4.1	$2.53\times10^8 \cdot T^{48} \cdot \exp(-1700/T)$	0.5	27
$H_2+HO_2 = OH+H_2O$	0.25–3	$6.5\times10^{11} \cdot \exp(-9400/T)$	1.0	28
$H_2+HO_2 = H_2O_2+H$	0.3–2.5	$3.01\times10^{13} \cdot \exp(-13100/T)$	0.5	29
$H_2+H_2O_2 = H_2O+OH+H$	0.5–3	$8.69\times10^{12} \cdot T^{0.5} \cdot \exp(-18347/T)$	–	30
$O_2+H = OH+O$	0.3–5.3	$8.65\times10^{14} \cdot T^{-0.24} \cdot \exp(-8200/T)$	0.1	31
$O_2+O_2 = O_3+O$	0.25–3	$1.2\times10^{13} \cdot \exp(-50500/T)$	0.6	32
$O_2+OH = O+HO_2$	0.3–2.5	$2.23\times10^{13} \cdot \exp(-26500/T)$	0.5	33
$O_2+OH = H+O_3$	0.25–3	$4.4\times10^7 \cdot T^{1.44} \cdot \exp(-38600/T)$	2.0	34
$O_2+HO_2 = OH+O_3$		No recommendation		35
$O_3+O = O_2+O_2$	0.2–1	$4.82\times10^{12} \cdot \exp(-2060/T)$	0.3	36
$O_3+H = OH+O_2$	0.2–2	$6.87\times10^{13} \cdot \exp(-437/T)$	0.7	37
$OH+O = H+O_2$	0.16–2.5	$8.91\times10^{12} \cdot \exp(251/T)$	0.3	38
$OH+H = O+H_2$	0.3–2.5	$4.88\times10^3 \cdot T^{2.8} \cdot \exp(-1950/T)$	0.3	39
$OH+OH = H_2O+O$	0.25–4.1	$1.5\times10^9 \cdot T^{1.14} \cdot \exp(-50/T)$	0.2	40
$OH+OH = H_2+O_2$	0.25–3	$1.7\times10^{13} \cdot \exp(-24100/T)$	0.8	41
$OH+OH = H+HO_2$	0.25–2.5	$1.2\times10^{13} \cdot \exp(-20200/T)$	1.0	42
$OH+O_3 = HO_2+O_2$	0.22–2.5	$9.6\times10^{11} \cdot \exp(-1000/T)$	0.6	43
$OH+H_2O = H_2+HO_2$	0.25–3	$7.9\times10^9 \cdot T^{0.43} \cdot \exp(-36100/T)$	1.4	44

$OH+H_2O = H+H_2O_2$	0.4–1	$2.4\times10^{14}\cdot exp(-40500/T)$	1.0	45
$OH+HO_2 = H_2O+O_2$	0.25–4.1	$2.85\times10^{13}\cdot exp(250/T)$	0.13	46
$OH+H_2O_2 = H_2O+HO_2$	0.3–1.45	$4.46\times10^{12}\cdot exp(-477/T)$	0.5	47
$H_2O+O = H+HO_2$		No recommendation		48
$H_2O+O = OH+OH$	0.25–3	$5.75\times10^{13}\cdot exp(-9052/T)$	0.2	49
$H_2O+H = H_2+OH$	0.5–2.5	$1.87\times10^{14}\cdot exp(-10433/T)$	0.3	50
$H_2O+O_2 = OH+HO_2$	0.5–3	$5.6\times10^{13}\cdot T^{0.17}\cdot exp(-36600/T)$	1.5	51
$H_2O+O_2 = H_2O_2+O$	0.5–2.5	$3.4\times10^{10}\cdot T^{0.52}\cdot exp(-44800/T)$	1.4	52
$H_2O+HO_2 = OH+H_2O_2$	0.3–2.5	$2.8\times10^{13}\cdot exp(-16500/T)$	0.3	53
$HO_2+O = OH+O_2$	0.22–2.5	$1.75\times10^{13}\cdot exp(200/T)$	0.3	54
$HO_2+H = OH+OH$	0.3–4.1	$1.69\times10^{14}\cdot exp(-440/T)$	0.4	55
$HO_2+H = O+H_2O$	0.25–1	$2.55\times10^{13}\cdot exp(-704/T)$	0.9	56
$HO_2+H = H_2+O_2$	0.25–2	$2.39\times10^{13}\cdot T^{0.09}\cdot exp(-710/T)$	0.2	57
$HO_2+O_3 = OH+2O_2$	0.2–1	$1.66\times10^{11}\cdot T^{-0.284}\cdot exp(-1000/T)$	0.45	58
$HO_2+HO_2 = H_2O_2+O_2$	0.3–2.5	1.8×10^{12}	0.5	59
$H_2O_2+O = OH+HO_2$	0.28–1	$1.08\times10^{12}\cdot exp(-2000/T)$	0.35	60
$O+ H_2O_2 = H_2O+O_2$	0.3–2.5	$8.4\times10^{11}\cdot exp(-2130/T)$	1	61
$H+H_2O_2 = H_2O+OH$	0.3–1	$1.02\times10^{13}\cdot exp(-1800/T)$	0.3	62
$H+H_2O_2 = HO_2+H_2$	0.3–1	$1.69\times10^{12}\cdot exp(-1890/T)$	0.3	63
$H_2O_2+O_2 = HO_2+HO_2$	0.3–2.5	$5.42\times10^{13}\cdot exp(-20000/T)$	0.7	64

Table 4. Reactions with electronically excited species

Reaction	ΔT, 10^3 K	k, cm^3/mol/s	Δlg k	Note
OH+OH = O*+H$_2$O	0.5–2.5	$1.0\times10^{13}\cdot\exp(-14100/T)$	–	66
HO$_2$+H=O*+H$_2$O	1–2.5	$1.7\times10^{12}\cdot T^{0.46}\cdot\exp(-678/T)$	–	67
O*+H$_2$=OH+H	0.2–0.5	1.0×10^{14}	0.25	68
O*+H$_2$=OH*+H	1–2.5	$2.0\times10^{14}\cdot\exp(-25000/T)$	–	69
O*+H$_2$O=2OH	0.2–0.35	1.32×10^{14}	–	70
O*+O$_3$=2O+O$_2$	0.2–1	7.94×10^{13}	–	71
O*+O$_2$*=O+O$_2$	0.29–0.3	6.03×10^{12}	–	72
2O$_2$*=2O$_2$	0.5–2.5	$7.5\times10^8\cdot\exp(-1180/T)$	–	73
O$_2$*+O$_2$=O$_3$+O	0.3–2.5	$1.2\times10^{13}\cdot\exp(-39604/T)$	–	74
O$_2$*+O$_3$=2O$_2$+O	0.28–2	$3.13\times10^{13}\cdot\exp(-2840/T)$	–*)	75
O$_2$*+H=OH+O	0.25–2.5	$1.1\times10^{14}\cdot\exp(-3188/T)$	–	76
OH+O=O$_2$*+H	0.3–2.5	$5.8\times10^{12}\cdot\exp(-6224/T)$	–	77
O$_2$*+H$_2$=2OH	0.25–2.5	$1.7\times10^{15}\cdot\exp(-17000/T)$	–	78
O$_2$*+H$_2$=H$_2$O+O*	0.5–2.5	$3.5\times10^{13}\cdot\exp(-20000/T)$	–	79
O$_2$*+H$_2$=HO$_2$+H	0.3–2	$2.49\times10^{12}\cdot\exp(-18234/T)$	–	80
H+HO$_2$=O$_2$*+H$_2$	0.27–2.5	$2.0\times10^{12}\cdot\exp(-293.4/T)$	–	81
O$_2$*+OH=H+O$_3$	0.25–2.5	$4.4\times10^7\cdot T^{1.44}\cdot\exp(-27225/T)$	–	82
O$_2$*+OH=O+HO$_2$	0.25–2.5	$1.3\times10^{13}\cdot\exp(-17000/T)$	–	83
O$_2$*+H$_2$O=HO$_2$+OH		No recommendation		84
O$_3$+OH=HO$_2$+O$_2$*	0.25–2.5	$4.8\times10^{11}\cdot\exp(-1000/T)$	–	85
O$_3$+HO$_2$=OH+O$_2$+O$_2$*	0.25–2.5	$1.0\times10^{10}\cdot\exp(-1000/T)$	–	86
HO$_2$+HO$_2$=H$_2$O$_2$+O$_2$*	0.25–2.5	$0.9\times10^{13}\cdot\exp(-500/T)$	–	87
H$_2$O$_2$+O=H$_2$O+O$_2$*	0.25–2.5	$4.2\times10^{11}\cdot\exp(-2130/T)$	–	88
O$_3$+H=OH* +O$_2$	0.25–2.5	$9.5\times10^{11}\cdot T^{0.85}\cdot\exp(-7900/T)$	–	89
OH* +O$_2$=O$_3$+H	0.5–2.5	$1.16\times10^{12}\cdot T^{0.5}$	–	90
H$_2$+O$_3$=HO$_2$+OH*	0.5–2.5	$1.0\times10^{12}\cdot\exp(-35100/T)$	–	91
H$_2$+HO$_2$=H$_2$O+OH*	0.25–2.5	8×10^9	–	92

*) See Comments

Table 5. Reactions of quenching

Reaction	ΔT, 10^3 K	M	k, cm^3/mol/s	Δlg k	Note
O_2*+M = O_2+M	0.5–2	O_2	1.0×10^6	–	97
	0.5–2	H_2	2.7×10^6	–	97
	0.5–2	O, H	4.2×10^8	–	97
	0.5–2	O_3	2.4×10^9	–	97
	0.5–2	H_2O, HO_2, OH, H_2O_2	3.4×10^6	–	97
	0.298	N_2	2.5×10^5	–	97
	0.298	Ar	$< 5 \times 10^3$	–	97
O*+M = O+M	0.2–0.35	O_2	$1.93 \times 10^{13} \cdot \exp(-67/T)$	–	98
	0.1–0.35	N_2	$1.1 \times 10^{13} \cdot \exp(-107/T)$	–	98
	0.298	O	3.0×10^{12}	0.3	98
	0.11–0.33	Ar	3.0×10^{11}	–	98
OH*+M = OH+M	0.5–1	O_2, H_2	$2.9 \times 10^{11} \cdot T^{0.5}$	–	99
	0.5–1	H_2O	$5.8 \times 10^{12} \cdot T^{0.5}$	–	99
	0.5–1	Ar	$2.9 \times 10^9 \cdot T^{0.5}$	–	99
$OH^* \rightarrow OH + h\nu$	–	–	For $v'=0$ lifetime $\tau =700$ ns, for $v'=2$ lifetime $\tau =90$ ns, for $v'=1$ – see comments *)	–	93
$O_2^* \rightarrow O_2 + h\nu$	–	–	$\tau = 3946$ s		94

*) See Comments

Comments

1. $H_2 + M = 2H + M$

a) $M = Ar, N_2$

The recommendation is given in [1].

b) $M = H_2, O_2$

The recommendation for $M = H_2$ is given in [1]. The same value is taken for $M = O_2$. The category of recommendation is "ID".

c) $M = H_2O$

The rate constant obtained in [2] is recommended.

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Cohen N., Westberg K.R. // J.Chem.Phys.Ref.Data. Vol.12. P.531 (1983).

2. $O_2 + M = 2O + M$

a) $M = Ar$

The recommended rate constant is obtained as a result of statistical data processing on the works [1,2].

b) $M = O_2, O$

The recommendation is given in [3].

c) $M = H_2O, O_3$

The recommendation is obtained in [4].

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1. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.
2.   Jerig L., Thielen K., Roth P.// AJAA J. 1991. Vol.29 (7). pp.11–39.
3. Baulch D.L., Drysdale D.D., Duxbury J., Grant S.J.Evaluated Kinetic Data for High Temperature Reactions. Vol.3. London. Butterworths. 1976.
4. Makarov V.N, Shatalov O.P. // Fluid Dynamics. 1994. № 6. pp.139–148 (in Russian).

3. $O_3 + M = O_2 + O + M$

a) $M = Ar$

The recommendation is given in [1]. This recommended value coincides with the recommendations of the works [2,3].

b) $M = O, O_2$

The recommendation is given in [2]. The category of recommendation is "ID".

c) $M = O_3$

The recommendation is given in [2]. The category of recommendation is "ID".

d) $M = N_2$

The recommendation is given in [3]. The category of recommendation is "ID".

----
1. Baulch D.L., Drysdale D.D., Duxbury J., Grant S.J.Evaluated Kinetic Data for High Temperature Reactions. Vol.3. London. Butterworths. 1976. 593 p.
2. Makarov V.N., Shatalov O.P. // Fluid Dynamics. 1994. № 6. pp.139-148 (in Russian).
3. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

4. $OH + M = O + H + M$

$M = Ar, O_2, N_2$

The data [1–3] agree with each other. The rate constant obtained in [3] is recommended.

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
2. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
3. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

5. $H_2O + M = OH + H + M$

a) $M = Ar$

The recommendation is given in [1].

b) $M = N_2$

The recommendation is given in [2].

c) $M = O_2$

The recommendation is given by analogy with the data for $M = N_2$ in [2]. The category of recommendation is "ID".

d) $M = H_2O_2$

The recommendation is given in [3].

----
1. Dougherty E.P., Rabitz H. // J.Chem.Phys.1980. Vol.72 (12). P. 6571.
2. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
3. Warnatz J. Rate coefficients in the C/H/O system. // "Combustion Chemistry", ed. W.C. Gardiner, pub. Springer-Verlag, NY, 1984.

6. $HO_2 + M = H + O_2 + M$

a) $M = Ar$

The recommendation is given in [1]. The same data are presented in [2,3].

b) $M = N_2$

The recommendation is given using data [2,3].

c) $M = O_2$

The recommendation is given by analogy with the data for $M = N_2$. The category of recommendation is "ID".

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1. Baulch D.L., Drysdale D.D., Horne D.G. Evaluated Kinetic Data for High Temperature Reactions. Vol.1. Homogeneous gas phase reactions of the H_2-O_2 system. London. Butterworths. 1972.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA. .
3. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

7. $HO_2 + M = H + O_2{}^* + M$

The recommendation is given in [1]. Collisional partner M is unidentified.. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

8. $H_2O_2 + M = OH + OH + M$

a) $M = Ar, N_2$

The recommendation is given in [1,2].

b) $M = H_2$

The rate constant obtained in [3] is recommended. The category of recommendation is "ID".

c) $M = H_2O_2$

The recommendation is given using [4]. The category of recommendation is "ID".

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1. Baulch D.L., Cobos C.J., Cox R.A. et al.//Combustion and Flame. 1994. Vol.98. P.59.
2. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P.6571.
3. Screbkov O.V., Karkach S.P. 2001. Private communication.
4. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA. .

9. $HO_2 + HO_2 + M = H_2O_2 + O_2 + M$

$M = N_2, O_2$

The recommendation is given in [1].

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. pp.1329–1499.

10. $H + H + M = H_2 + M$

a) $M = Ar, H_2$

The recommendation is given in [1]

b) $M = H, H_2O$

The recommendation is given in [2].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Cohen N., Westberg K.R. // J. Chem. Phys. Ref. Data. Vol.12. P531 (1983).

11. $O + O + M = O_2 + M$

a) $M = Ar$

The recommendation is given in [1].

b) $M = N_2$

The recommendation is given in [2].

c) $M = O, O_2, O_3$

The recommendation is given in [3].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
2. Dougherty E.P., Rabitz H. // J. Chem. Phys. 1980. Vol.72 (12). P. 6571.
3. Makarov V.N., Shatalov O.P.//J.Fluid dynamics. 1994. № 6. pp.139–148 (in Russian).

12. $O + O_2 + M = O_3 + M$

a) $M = Ar$

The recommendation is given in [1].

b) $M = N_2$

Recommendation is obtained by statistical processing of the data [2, 3].

c) $M = O_2$

Recommendation is obtained by statistical processing of the data [3, 4].

d) $M = O, O_3$

The recommendation is given in [4].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
2. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
3. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
4. Makarov V.N., Shatalov O.P.//J. Fluid dynamics. 1994. № 6. pp.139-148 (in Russian).

13. $O + O_2^* + M = O_3 + M$

The rate constant obtained in [1] is recommended. Collisional partner M is unidentified. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

14. $O + H + M = OH + M$

The rate constant obtained in [1] is recommended. Collisional partner M is unidentified. The category of recommendation is "ID".

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1. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.

15. $O + H + M = OH^* + M$

$M = Ar, H_2, O_2, OH$

The rate constant obtained in [1] is recommended The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).

16. $O^* + H + M = OH^* + M$

a) $M = Ar, H_2, O_2$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

----

1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp. 1–4 (in Russain).

17. $H + OH + M = H_2O + M$

a) $M = Ar$

The recommendation is given in [1].

b) $M = N_2$

The recommendation is given in [1].

c) $M = H_2$

The recommendation is given in [2]. There are also taken into account the results of the work [3]. The category of recommendation is "ID".

d) $M = OH$

The recommendation is given in [4].

e) $M = H_2O$

The recommendation is given in [1].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Skrebkov O.V., Karkach S.P., 2001. Private communication.
3. Getzinger R.W., Blaair L.S. // Combust. Flame. 1969. Vol.13. pp.271–284.
4. Davies M.G., McGregor W.K., Mason A.A. // J.Chem.Phys. 1974. Vol.61. P.1352.

18. $H + O_2 + M = HO_2 + M$
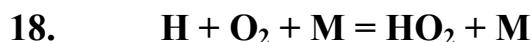
a) $M = Ar$

The recommendation is given in [1]. There are also taken into account the results [2,3].

b) $M = N_2$

 The recommendation is obtained by statistical processing of the data of reviews [1,4,5].

c) $M = H_2$

The recommendation is given in [1].

d) $M = O_2$

The recommendation is given using the data [6−8]. The category of recommendation is "ID".

e) $M = H_2O$

The recommendation is given in [9].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59−79.
2. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
3. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.
4. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.
5. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
6. Skrebkov O.V., Karkach S.P., 2001. Private communication.
7. Getzinger R.W., Blaair L.S. // Combust. Flame. 1969. Vol.13. pp.271−284.
8. Peeters J., Mahnen G. // Symp. Int. Combustion. Proc. 14, P.133 (1973).
9. Baulch D.L., Cobos C.J., Cox R.A. et al. // J. Phys. Chem. Ref. Data. 1992. Vol.21. pp.411−736.
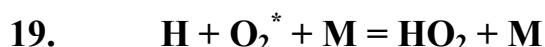
19. $H + O_2{}^* + M = HO_2 + M$

The recommendation is given in [1]. Collisional partner M is unidentified. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // J.Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17−25 (in Russian).

20. $OH + OH + M = H_2O_2 + M$

a) $M = Ar$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

b) $M = N_2$

The recommendation is given in [2, 3].

c) $M = H_2O$

The recommendation is given in [2}.

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

2. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
3. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.

21. $O + H_2 = OH + H$

The recommendation is given in [1]. There are also taken into account the results [2].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.

22. $H_2 + O_2 = O + H_2O$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).

23. $H_2 + O_2 = H + HO_2$

Recommendation is obtained by statistical processing of experimental results of five works cited in [1] and the data [2].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.

24. $H_2 + O_2 = OH + OH$

Recommendation is obtained by statistical processing of the data of seven experimental works cited in [1].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA. .

25. $H_2 + 2O_2 = 2HO_2$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).

26. $H_2 + O_3 = HO_2 + OH$

Recommendation is not proposed because of conflicting data of the works [1,2]:
$k = 6 \times 10^{10} \cdot \exp(-10000/T)$ cm^3/mol/s [1], $k = 1 \times 10^{11} \cdot \exp(-35000/T)$ cm^3/mol/s [2]. Another data are absent.

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25.
2. Skrebkov O.V., Karkach S.P., 2001. Private communication.

27. $H_2 + OH = H + H_2O$

Recommendation was obtained by statistical processing of experimental results cited in [1]. There were also taken into account the high-temperature data [2] and recommendations [3].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.
3. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.

28. $H_2 + HO_2 = OH + H_2O$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

29. $HO_2 + H_2 = H_2O_2 + H$

Recommendation was obtained by statistical processing of experimental results of four works cited in [1] and the data [2].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

30. $H_2 + H_2O_2 = H_2O + OH + H$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID". In [2] there is taken the rate constant $k = 0.35$ cm^3 /mol/s at $T = 741$ K for reaction $H_2 + H_2O_2 = 2OH + H_2$ [3].

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
3. Baldwin R.R., Booth D., Brattan D. // Can. J. Chem.1961. Vol.39. P.2130.

31. $H + O_2 = OH + O$

Recommendation is obtained by statistical processing of experimental results cited in [1] and the data [2.3].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.
3. Du H., Hessler J.P. // J.Chem.Phys. 1992. Vol.96 (2). pp.1077–1091.

32. $O_2 + O_2 = O + O_3$

The recommendation is given in [1]. This recommended rate constant is similar to the data [2,3].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
2. Benson S.W., Axwworthy A.E. // J.Chem.Phys. 1957. Vol.26. pp.1718–1726.
3. Makarov V.N., Shatalov O.P.//J.Fluid Dynamics. 1994. №6. pp.139–148 (in Russian).

33. $O_2 + OH = O + HO_2$

The recommendation is given in [1].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

34. $O_2 + OH = H + O_3$

The recommendation is given in [1]. The category is "ID" because of great uncertainty of rate constant.

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

35. $O_2 + HO_2 = OH + O_3$

Recommendation is not proposed because of conflicting data [1,2]: $k = 9 \times 10^8$ cm^3/mol/s [1], $k = 2.14 \times 10^{12} \cdot \exp(-22000/T)$ cm^3/mol/s [2].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
2. Screbkov O.V., Karkach S.P., 2001. Private communication.

36. $O + O_3 = O_2 + O_2$

The recommendation is given in [1]. The recommendation is similar to the rate constant obtained by statistical processing of experimental data from database [2].

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.

37. $H + O_3 = OH + O_2$

The recommendation is taken as a result of statistical processing of experimental data cited in [1].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.

38. $O + OH = O_2 + H$

The recommendation is taken as a result of statistical processing of experimental data cited in [1].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.

39. $OH + H = O + H_2$

The recommendation is given in [1].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

40. $OH + OH = H_2O + O$
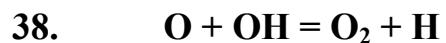
The recommendation is given in [1]. The temperature range was extended to T=4100K taking into account the data [2].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45.

41. $OH + OH = H_2 + O_2$

The recommendation is given in [1].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

42. $OH + OH = HO_2 + H$

The recommendation is given in [1].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

43. $OH + O_3 = HO_2 + O_2$

The recommendation is given in [1].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

44. $OH + H_2O = H_2 + HO_2$

The recommendation is given in [1].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

45. $OH + H_2O = H + H_2O_2$

The recommendation is given in [1].

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

46. $OH + HO_2 = H_2O + O_2$
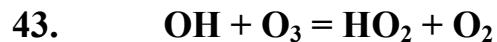
The recommendation is taken as a result of statistical processing of data [1-4].

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.
2. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. P.59-79.
3. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
4. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45

47. $OH + H_2O_2 = H_2O + HO_2$

The recommendation is a result of statistical processing of experimental data cited in [1]. Recommended rate constant agrees very well with low-temperature data [2]. At $T = 2000$ K recommended rate constant differs by factor 1.4 from recommendation [3].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
3. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. P.59-79.

48. $H_2O + O = H + HO_2$
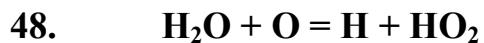
Recommendation is not proposed because of conflicting data on the reaction. The rate constant is very small (for example, see [1]: $k = 4.4\times10^6$ cm^3/mol/s, $T = 298$ K).

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1. Hack W., Preuss A.V., Wagner H.G. et al. // Ber. Bunsenges. Phys. Chem.1979. Vol.83. P.212).

49. $H_2O + O = OH + OH$
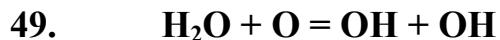
The recommendation is a result of statistical processing of experimental data cited in [1]. Its value agrees well with the data [2–5].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
3. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
4. Warnatz J. Rate coefficients in the C/H/O system. // "Combustion Chemistry", ed. W.C. Gardiner, pub. Springer-Verlag, NY, 1984.
5. Harding L.B., Wagner A.F. // Symp. Int. Combust., Proc. 22, pp.983–989 (1989) (calculation by transition state theory).

50. $H_2O + H = H_2 + OH$

The recommendation is a result of statistical processing of experimental data of great number of works cited in [1]. Its value agrees well with the data [2-4].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Baulch D.L., Cobos C.J., Cox R.A. et al. Evaluated kinetic data for combustion modelling. // J. Phys. Chem. Ref. Data. 1992. Vol.21. pp.411–736.
3. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
4. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

51. $H_2O + O_2 = OH + HO_2$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

52. $H_2O + O_2 = H_2O_2 + O$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

53. $HO_2 + H_2O = H_2O_2 + OH$

The rate constant obtained in [1] is recommended.

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1. Lloyd A.C. // J. Chem. Kinet. 1974. Vol.6. pp.169–228.

54. $HO_2 + O = OH + O_2$

The recommendation is given in [1].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

55. $HO_2 + H = OH + OH$

The recommendation was given in according to the data [1,2]. The temperature range was extended to $T = 4100$ K taking into account the data [3].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. P.59.
2. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
3. Koike T. // Memoirs of NDA. Japan. March 1994. Vol.33. P.45 .

56. $HO_2 + H = O + H_2O$

The recommendation is taken as a result of statistical processing of the data [1,2].

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.
2. Starik A.M., Titova N.S.. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

57. $HO_2 + H = H_2 + O_2$

The recommendation is given in [1]. Recommended rate constant is less by factor 1.5 than the value obtained by statistical processing of experimental data of works cited in [2].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. P.59.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA.

58. $HO_2 + O_3 = 2O_2 + OH$

The recommendation is a result of statistical processing of the data [1-4].

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329-1499.
2. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.
3. DeMoore W.B., Sander S.P., Golden D.M., et al. // JPL Publication. 1997. 97- 4.
4. Lloyd A.C. // J. Chem. Kinet. 1974. Vol.6. pp.169–228.

59. $HO_2 + HO_2 = H_2O_2 + O_2$

The recommendation is given in [1]. In [2] more fifty experimental works and reviews are presented but all the data are very contradictory.

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.
2. NIST Chemical Kinetics Database (Standard Reference Database 17-2Q98. 1998.- NIST. Gaithersburg. MD. USA).

60. $O + H_2O_2 = OH + HO_2$

The recommendation is a result of statistical processing of the data [1–3].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. P.59.
2. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
3. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

61. $O + H_2O_2 = H_2O + O_2$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Dougherty E.P., Rabiz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

62. $H + H_2O_2 = H_2O + OH$

The recommendation is given in [1].

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59−79.

63. $H + H_2O_2 = HO_2 + H_2$

The recommendation is given in [1]. Its value coincides with the experimental data cited in [2].

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1. Baulch D.L., Cobos C.J., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1992. Vol.21. P.411.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA

64. $O_2 + H_2O_2 = HO_2 + HO_2$

The recommendation is given in [1].

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1. Tsang W., Hampson R.F. // J. Phys. Chem. Ref. Data. 1986. Vol.15. P.1087.

65. $O_3 + M = O_2(^1\Delta) + O + M$

The recommendation is given in [1]. Collisional partner M is unidentified. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17−25 (in Russian).

66. $OH + OH = O(^1D) + H_2O$
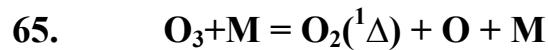
The rate constant obtained in [1] is recommended. Evaluation of high limit of rate constant. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

67. $HO_2 + H = O(^1D) + H_2O$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).

68. $O(^1D) + H_2 = OH + H$
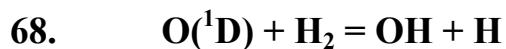
The recommendation is given according to [1]. At $T = 200–500$ K the uncertainty is: $\Delta \lg k = 0.25$. At $T = 500–2000$ K the category of recommendation is "ID".

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1. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA

69. $O(^1D) + H_2 = OH(^2\Sigma) + H$
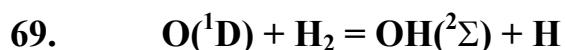
Recommendation is the high limit of rate constant given in [1]. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

70. $O(^1D) + H_2O = OH + OH$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.

71. $O(^1D) + O_3 = O + O + O_2$
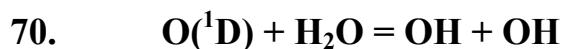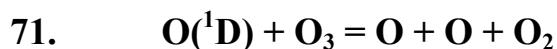
The recommendation is given using data [1,2]. The category of recommendation is "ID".

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
2. Skrebkov O.V., Karkach S.P., 2001. Private communication.
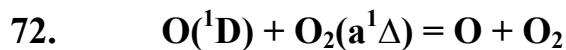
72. $O(^1D) + O_2(a^1\Delta) = O + O_2$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

73. $2O_2(a^1\Delta) = 2O_2$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

74. $O_2(a^1\Delta) + O_2 = O_3 + O$

The recommendation is given in [1]. The category of recommendation is "ID".

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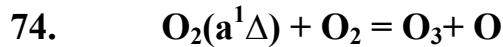
1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. C.17-25 (in Russian).

75. $O_2(a^1\Delta) + O_3 = O_2 + O_2 + O$
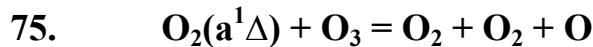
The recommendation is given using data [1,2]. The uncertainty is $\Delta\lg k = 0.1$ at $T = 280$–400 K. At $T > 400$ K the category of recommendation is "ID".

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1. Baulch D.L., Cobos C.J., Cox R.A. et al. // Combustion and Flame. 1994. Vol.98. pp.59–79.
2. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.

76. $O_2(a^1\Delta) + H = OH + O$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Basevich V.Ja., Beljaev A.A. // Chimicheskaya fizika. 1989. Vol.8 (8). P.1124 (in Russian).

77. $OH + O = O_2(a^1\Delta) + H$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Basevich V.Ja., Beljaev A.A. // Chimicheskaya fizika. 1989. Vol.8 (8). P.1124 (in Russian).

78. $O_2(a^1\Delta) + H_2 = OH + OH$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

79. $O_2(a^1\Delta) + H_2 = H_2O + O(^1D)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

80. $O_2(a^1\Delta) + H_2 = HO_2 + H$
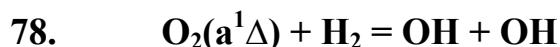
The rate constant obtained in [1] is recommended. The rate constant was calculated by the method «bond energy – bond order». The category of recommendation is "ID".

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1. Mayer S.W., Schieler L. // J. Chem. Phys. 1968. Vol.72. P.2628.

81. $HO_2 + H = O_2(a^1\Delta) + H_2$

The rate constant obtained in [1] is recommended. The data obtained in [2] are greater than recommendation by factor 2.5 at T=273K. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.
2. Kulaguin Ju.A. Kinetics of processes in gases under making of nonequilibrium by chemical and gasdynamic methods. Dissertation... Dr. on Sciences, 1996. Central Scientific-research Institute of Chemistry and Mechanics. Moscow (Russia).1996.

82. $O_2(a^1\Delta) + OH = H + O_3$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

83. $O_2(a^1\Delta) + OH = O + HO_2$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

84. $O_2(a^1\Delta) + H_2O = HO_2 + OH$

The recommendation is not proposed. The data [1, 2] differ by several orders:
$k = 1.5 \times 10^{15} \cdot T^{0.5} \cdot \exp(-25521/T)$ cm^3/mol/s [1], $k = 9.9 \times 10^{12} \cdot \exp(-25830/T)$ cm^3/mol/s [2].

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).
2. Mayer S.W., Schieler L. // J. Chem. Phys. 1968. Vol.72. P.2628 (calculations by the method «bond energy – bond order»)

85. $O_3 + OH = HO_2 + O_2(a^1\Delta)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

86. $O_3 + HO_2 = OH + O_2 + O_2(a^1\Delta)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

87. $HO_2 + HO_2 = H_2O_2 + O_2(a^1\Delta)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

88. $H_2O_2 + O = H_2O + O_2(a^1\Delta)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

89. $O_3 + H = OH(^2\Sigma) + O_2$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

90. $OH(^2\Sigma) + O_2 = O_3 + H$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

91. $H_2 + O_3 = HO_2 + OH(^2\Sigma)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P., 2001. Private communication.

92. $H_2 + HO_2 = H_2O + OH(^2\Sigma)$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya chimiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).

93. $OH(A^2\Sigma) \rightarrow OH + h\nu$

In classic work [1] the life time of $OH(A^2\Sigma)$ was studied on vibrational levels $v' = 0,1,2$. The levels with $v' = 0$ and 1 are predissociated partially: for $v' = 0$ with rotational quantum numbers $N > 23$ and for $v' = 1$ with rotational quantum numbers $N > 14$. All the rotational levels appurtenant to $v' = 2$ are predissociated completely. Therefore life time τ for electronic state $A^2\Sigma$ greatly depends on vibrational and rotational level. In the work it was defined that $\tau(v' = 0) \sim 700$ ns, $\tau(v' = 2) \sim 90$ ns.

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1. Brzozowki J., Erman P., Lyyra M. // Physica Scripta. 1978. Vol.17 (5). P.507)

94. $O_2(^1\Delta) \rightarrow O_2 + h\nu$
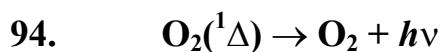
The life time of electronic state $O_2(^1\Delta)$ was evaluated by *ab initio* calculations in [1]. It was found that $\tau = 3946$ s.

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1. Zhu J.-K., Pan Y.-K. // Chem. Phys. Lett. 1981. Vol.78 (1). pp.129–130.
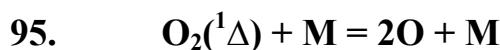
95. $O_2(^1\Delta) + M = 2O + M$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Starik A.M., Titova N.S. // Chimicheskaya fizika. 2001. Vol.20. № 5. pp.17–25 (in Russian).

96. $OH + O + M = HO_2 + M$

The recommendation is given in [1]. The category of recommendation is "ID".

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1. Dougherty E.P., Rabitz H. // J.Chem.Phys. 1980. Vol.72 (12). P. 6571.

97. $O_2(a^1\Delta) + M = O_2 + M$
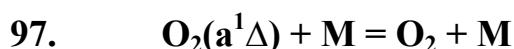
a) $M = O, H, O_2, H_2, OH, O_3, H_2O, HO_2, H_2O_2$

The recommendation is given in [1]. The category of recommendation is "ID".

b) $M = Ar, N_2$

The recommendation is given using [2]. The category of recommendation is "ID".

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1. Kulaguin Ju.A. Kinetics of processes in gases under making of nonequilibrium by chemical and gasdynamic methods. Dissertation… Dr. on Sciences, 1996. Central Scientific-research Institute of Chemistry and Mechanics. Moscow (Russia).1996.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA

98. $O(^1D) + M = O + M$

a) $M = O_2, N_2$

The recommendation is given in [1]. The category of recommendation is "ID".

b) $M = Ar, O$

The recommendation is given using [2]. For M = Ar the category of recommendation is "ID".

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1. Atkinson R., Baulch D.L., Cox R.A., et al. // J. Phys. Chem. Ref. Data. 1997. Vol.26. P.1329.
2. NIST Chemical Kinetics Database. Standard Reference Database 17-2Q98. 1998. - NIST. Gaithersburg. MD. USA

99. $OH^* + M = OH + M$
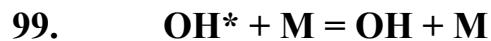
$M = Ar, O_2, H_2, H_2O$

The rate constant obtained in [1] is recommended. The category of recommendation is "ID".

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1. Skrebkov O.V., Karkach S.P. et al. // Doklady akademii nauk. Seriya "Fizicheskaya himiya". 2002. Vol.383. № 6. pp.1–4 (in Russain).