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Expert evaluation of kinetic data for use in research on atmospheric modelling

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ABSTRACT. The development of data banks on chemical kinetics and photochemistry for use in modelling the atmosphere is examined. A table representing a compilation of data on the chemistry of the formation of stratospheric ozone in which the reactions are grouped into families (O_x, HO_x, NO_x, ClO_x, and organic reactions) is published. An approach to the selection of the recommended values of kinetic and photochemical quantities, developed by CODATA/IUPAC experts, is described in detail. The review is completed by a brief discussion of the immediate prospects for the development of expert evaluations of data for atmospheric chemistry.

The bibliography includes 40 references.

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I. Introduction

Studies on expert evaluations of kinetic data for use in atmospheric modelling were initiated in 1971 by the Information Centre on Chemical Kinetics at the National Bureau of Standards (Washington). They were stimulated by the suggestion that, as a consequence of chemical reactions involving nitric oxide ejected by supersonic aeroplanes, a significant decrease in the ozone content of the stratosphere might take place[1,2]. Studies on expert evaluations of kinetic data at the National Bureau of Standards soon included in the Program for the Evaluation of Influences on the Climate (Department of Transportation of the USA). This program was started in 1970–1971 with the aim of determining the possible ecological consequences of the pollution of the stratosphere by aeroplane exhausts. A characteristic feature of the program involved studies designed to estimate the photochemical and kinetic parameters of stratospheric reactions: these investigations were published in the open press and also in the reports of the National Bureau of Standards[3,4].

In September 1975 the CODATA Expert Panel on Chemical Kinetics held an international symposium on "Kinetic Data for the Upper and Lower Atmosphere". This symposium and its published proceedings[5] constituted the cornerstone in establishing the importance of kinetic information for the chemistry of the atmosphere.

In 1976 the National Aeronautics and Space Administration of the USA (NASA) assumed the duty of assessing the influence of the released ureons on stratospheric ozone. The next landmark in the creation of surveys of data on atmospheric processes was the NASA publication 1010 "Chlorofluoromethanes and the Stratosphere"[6]. This publication became the first of the regular surveys of kinetic and photochemical data for stratospheric modelling which are prepared by the NASA Expert Panel, and is published by the Jet Propulsion Laboratory in Pasadena (California). Approximately one review has been published every 18 months in this series since 1977. Communication No. 9 has already been published and work of this kind is being continued.

Together with the start of the NASA publications, the necessity for organising an international Expert Panel for the preparation of surveys of kinetic parameters for reactions relevant to atmospheric chemistry was recognised. The principal feature of this approach was the global nature of the object of study. The CODATA Working Group on Chemical Kinetics has been newly created under the aegis of the International Council of Scientific Societies. The first publication of this international group[8] dates back to 1980. Supplements were issued in 1982, 1984, and 1989.[9] The last of these communications was prepared by the IUPAC Subcommittee for the evaluation of data for atmospheric chemistry which has replaced the CODATA Working Group and has continued to work on surveys of kinetic data.

The NASA Expert Panel and the CODATA/IUPAC Group have collaborated closely during the last 13 years. The NASA surveys are published more frequently and are aimed at stratospheric chemistry whereas the CODATA/IUPAC surveys include both stratospheric and tropospheric reactions. Both groups have prepared a general survey of data for inclusion in the report by the World Meteorological Organisation "the Stratosphere" [10].

The creation of these two independent Expert Panels, supplementing one another, has made it possible to solve the difficult problem of evaluating kinetic and photochemical data on a collective basis. The NASA Panel (USA) has at its disposal the national system for the dissemination of data whereas the IUPAC International Subcommittee has a broader base but publishes its surveys more rarely.

This communication considers the approach used and the results of the surveys of the IUPAC Subcommittee on Kinetic and Photochemical Data for Atmospheric Chemistry.

As an illustration, a list of data for one of the reactions is given and there is also a complete list of reactions together with the recommended rate constants and errors

II. Families of reactions in atmospheric chemistry

In 1930 Chapman put forward a photochemical theory of the formation of stratospheric ozone in reactions involving species containing oxygen alone[11,12]:

$$O_2 + h\nu \rightarrow O + O, \quad (1)$$

$$O + O_2 + M \rightarrow O_3 + M, \quad (2)$$

$$O_3 + h\nu \rightarrow O + O_2, \quad (3)$$

$$O + O_3 \rightarrow 2O_2. \quad (4)$$

These reactions constitute the basis of the O_x family. Reactions of vibrationally and electronically excited species were recently added to this family (see Section V).

The measurements of the rate constants for reaction (4) carried out in the 1950s showed that the reaction is much slower than had been believed at the time when Chapman proposed his theory. The concentration of ozone calculated on the basis of reactions (1)–(4) by the method of stationary concentrations proved to be higher than that observed in the atmosphere. In order to account for this discrepancy, Hunt[13] suggested that the HO_x species (H, HO, HO_2), first introduced by Bates and Nicolet[14], participate in the ozone destruction catalytic cycles:

$$H + O_3 \rightarrow HO + O_2, \quad (5)$$

$$\frac{HO + O \rightarrow H + O_2,}{\text{total } O + O_3 = 2O_2.} \quad (6)$$

$$HO + O_3 \rightarrow HO_2 + O_2, \quad (7)$$

$$\frac{HO_2 + O \rightarrow HO + O_2,}{O + O_3 = 2\,O_2.} \quad (8)$$

$$HO_2 + O_3 \rightarrow HO + 2\,O_2, \quad (9)$$

$$\frac{HO + O_3 \rightarrow HO_2 + O_2,}{O_3 + O_3 = 3\,O_2.} \quad (10)$$

Reactions (5)–(10) form part of the family of the HO_x reactions presented below in Table 2.

The next step in the development of the theory of the photochemical formation of ozone occurred at the beginning of the 1970s when Crutzen[1] proposed a catalytic cycle with participation of NO_x. Johnston[2] suggested soon afterwards that the nitrogen oxides from the exhausts of supersonic aeroplanes lead to the depletion of the ozone layer, which has serious consequences as a result of the increase in the transparency of the atmosphere to ultraviolet rays.

$$NO + O_3 \rightarrow NO_2 + O_2, \quad (11)$$

$$\frac{NO_2 + O \rightarrow NO + O_2,}{O + O_3 = 2\,O_2.} \quad (12)$$

The family of the NO_x reactions, presented below in Table 2, was thus introduced into consideration. It shows that there is an appreciable interaction between the catalytic NO_x cycle, the HO_x and ClO_x families (see below). One of the pathways in such interaction involves reactions which have a direct influence on the conversion of the NO_x and ClO_x species into other active forms, for example:

$$HO_2 + NO \rightarrow HO + NO_2, \quad (13)$$

$$ClO + NO \rightarrow Cl + NO_2. \quad (14)$$

The hypothesis by Molina and Rowland[15] that the chlorine atoms formed on photochemical decomposition of chlorofluorocarbons (CFC) in the upper atmosphere can lead to an appreciable destruction of ozone in the catalytic cycle

$$Cl + O_3 \rightarrow ClO + O_2, \quad (15)$$

$$\frac{ClO + O \rightarrow Cl + O_2,}{O + O_3 = 2\,O_2.} \quad (16)$$

made the problem of the decomposition of the ozone layer still more acute. Subsequently an appreciable number of supplementary reactions were added to the ClO_x family (see Table 2 below).

Chlorofluorocarbons accumulate rapidly in the atmosphere and, because of their long lifetime, it would be impossible to neutralise their influence in the foreseeable future. A need therefore arises for predictive mathematical models capable of describing the behaviour of atmospheric ozone now and in the future. Such models have been vigorously developed during the past 15 years. One-dimensional models with transport are being replaced nowadays by two-dimensional (width–height) models. Both types of models include 150 elementary gas phase chemical and photochemical reactions. The characteristics of these models as well as kinetic data banks have been periodically considered in reviews, so that the prediction of the changes in the ozone content rests on a reliable scientific basis.

The report[16] of a significant decrease in the amount of ozone during springtime over the Antarctic ("ozone hole") in 1985 was very unexpected. Models did not predict such changes. The subsequent vigorous field and laboratory studies revealed new chemical processes in the lower stratosphere. These include heterogeneous reactions on the surfaces of polar stratospheric clouds which are formed on condensation of water vapour with an admixture of nitric acid. These reactions convert a large proportion of chlorine into a catalytically active form. Thus it was shown that chlorine constitutes a serious threat to ozone. These studies led to attempts to replace the long-lived chlorofluorocarbons by substances with similar properties but more readily removed from the atmosphere, for example, by reaction with the HO radicals in the troposphere.

Tropospheric chemistry has become a rapidly developing field after it was suggested that there are high stationary concentrations of HO and HO_2 in the troposphere in the presence of sunlight.[17] Since HO radicals are highly reactive, the reactions with them constitute an important sink for the majority of trace impurities. Further progress in tropospheric chemistry is associated with the study of the photochemical formation of oxidants or smog. Demerjian et al.[18] were the first to formulate the mechanisms of the oxidation of hydrocarbons in the presence of NO_x with formation of ozone in polluted air. Kinetic data for the modelling of tropospheric chemistry are presented in Table 2 in the "Organic reactions" Section.

The complexity of both tropospheric and stratospheric chemistry requires accurate data for a multiplicity of elementary gas-phase reactions. Expert evaluation of data has played a major role in combining experimental and theoretical information. In the sections which follow in this review, an approach is described to the evaluation of data for atmospheric chemistry.

III. Format for the presentation of data

At the beginning of studies concerning the expert evaluation of chemical and photochemical data, the CODATA Working Group had to select a suitable format for the presentation of data. Previous reviews were either detailed, involving a detailed consideration of individual measurements, for example, the reviews on high-temperature kinetics[19], or were abbreviated, as in the early Tables of the National Bureau of Standards[4]. The CODATA Group selected an intermediate degree of detail: the experimental methods and conditions are indicated and the discrepancies between the results of different studies are discussed. This was achieved by employing the "list of data" approach in which information is compiled and discussed in a standardised form for each elementary reaction. The reactions were grouped in terms of the O_x, HO_x, NO_x, organic, SO_x, FO_x, ClO_x, BrO_x, and IO_x families.

IV. Compilation of lists of data

1. Thermal reactions

The list of data[19] is begun with the formation of the reaction equation taking into account all of its feasible pathways. Next, the enthalpy change at 298 K is quoted. The available kinetic data are presented in four sections—the rate constants obtained from absolute and relative measurements, branching parameters, and recommended constants with an indication of the Expert Panel.

Since all the reactions considered are elementary chemical processes, the expression for the rate of reaction is formulated in accordance with the reaction equation:

$$A + A \rightarrow B + C,$$
$$-1/2\frac{d[A]}{dt} = \frac{d[B]}{dt} = \frac{d[C]}{dt} = k[A]^2.$$

Thus the stoichiometric coefficient 2 for A appears in the denominator before the rate of change of [A] {it is equal to $2k[A^2]$} and in the power exponent in the right-hand side of the equation.

The rate constants for reactions are presented in the form of the simple Arrhenius equation: $k = A\exp(-B/T)$, where $B = E/R$ can be both positive and negative. For the pressure-dependent recombination and dissociation rate constants, a non-Arrhenius temperature variation is used, which is discussed in the next Section.

The kinetic data are provided with commentaries in which experimental details are described. The recommended rate constants are quoted for 298 K and also in the form of a temperature variation equation for the temperature range indicated. The errors in $\lg k$ at 298 K and in the values of E/R in the temperature range of the recommended rate constants are indicated. The choice of the recommended values is justified in the commentary and other relevant information is presented.

A typical list of data for the thermal reaction $HO + HCHO \rightarrow H_2O + HCO$ is presented in Table 1.

2. Recombination and dissociation reactions

The rates of recombination and dissociation reactions depend on the temperature T, the nature of the species, and the concentration of the third body M:

$$A + B + M \rightarrow AB + M.$$

Table 1. Typical list of data from a CODATA survey[9]

$HO + HCHO \rightarrow H_2O + HCO$, (1)
$HO + HCHO \rightarrow H + HCOOH$, (2)
$\Delta H°(1) = -135.3$ kJ mol^{-1},
$\Delta H°(2) = -91.5$ kJ mol^{-1}
The rate constant $k = k_1 + k_2$.

k, cm^3 s^{-1}	T, K	Refs.	Remarks**
Absolute measurement			
$(8.1\pm0.5)\cdot10^{-12}$	296	[20]	1
$(1.66\pm0.20)\cdot10^{-11}\exp(-86/T)$	296—576	[21]	2
$(1.25\pm0.11)\cdot10^{-11}$	298		
Relative measurements			
$(8.4\pm0.5)\cdot10^{-12}$	299	[22]	3
Branching parameters			
$k_1/k = 1.00\pm0.05$	296	[20]	1
$k_2/k < 0.02$	299	[22]	3
Values recommended previously			
$1.1\cdot10^{-11}$	200—425	[23]	4
$5.0\cdot10^{-11}\exp(-600/T)$	300—2500	[24]	5
$1.0\cdot10^{-11}$	228—426	[25]	6
$9.0\cdot10^{-12}$	228—426	[26]	7
$5.7\cdot10^{-15}T\,1.18\exp(225/T)$	300—1660	[27]	8
$1.0\cdot10^{-11}$	228—426	[28]	6
Recommended values*			
$1.1\cdot10^{-11}$	298	—	—
$1.6\cdot10^{-11}\exp(-110/T)$	230—580	—	—
$k_1/k = 1.0$	298	—	—

Reliability
$\Delta\lg k = \pm0.1$ at 298 K
Determination of errors
$\Delta(E/R) = \pm150$ K;
$\Delta(k_1/k) = \pm0.1$ at 298 K

* The recommended values were obtained by the method of least squares using the absolute rate constants determined in a number of investigations[20,21,30,31] and agreeing well with one another at room temperature. The results of relative measurements obtained in several investigations[22,29,34] correspond to the recommended values at 298 K. Analysis of the products[20,22] showed that at 298 K this reaction proceeds predominantly via pathway 1 with formation of H_2O + HCO.

** The figures in the remarks column have the following significance; (1) discharge flow—detection of HO and HCO radicals by the laser magnetic resonance method. The ratio k_1/k was obtained by comparing the amount of HCO formed with the amount of HO which had reacted; (2) laser photolysis—detection of HO by the laser-induced fluorescence method; (3) method of relative rates. The HO radicals were generated by the photolysis of $CH_3ONO-NO-$air and $C_2H_5ONO-NO-$air mixtures at an overall air pressure of 700 mmHg. The rates of disappearance of $H^{13}CHO$ and C_2H_4 were determined by IR spectroscopy. The rate constant ratio $k/k(HO + C_2H_4) = 0.99 \pm 0.06$ was converted into the absolute value assuming that $k(HO + C_2H_4) = 8.5 \times 10^{-12}$ cm^3 s^{-1} [26]. The ^{13}C isotope effect was neglected. The ratio $k_2/k = 0.02$ was estimated on the basis of the absence of $H^{13}COOH$ from the products; (4) obtained as the average of the rate constants determined in a number of studies[29—31]; (5) based mainly on rate constant data[30,32,33]; (6) the rate constant at 298 K is the mean of the absolute values determined in two studies[30,31]. These data do not indicate any temperature dependence of the rate constants; (7) obtained from values determined in a number of investigations[20,22,30,31] on the assumption that the rate constant is independent of temperature[24,30]; (8) based on a number of data[30—33].

The rate constants for such reactions should be expressed in a more complex form than the rate constants for simple bimolecular reactions. Recombination reactions are described in terms of a pseudo-second order law:

$$\frac{d[AB]}{dt} = k[A][B].$$

Here the second-order rate constant k depends on [M]. The low pressure limit for the third-order rate constant is characterised by a quantity k_0 proportional to [M]:

$$k_0 = \lim_{[M]\to 0} k([M]).$$

The high pressure limit (the bimolecular constant) is characterised by a quantity k_∞ which is independent of [M]:

$$k_\infty = \lim_{[M]\to \infty} k([M]).$$

For recombination reactions in the region of low pressures, Table 1 presents second-order rate constants expressed as the product of the third-order rate constant and the concentration of the third species. The transition between third- and second-order regions is described by the equation quoted for the decrease in k/k_∞ as a function of

$$k_0/k_\infty = [M]/[M]_c,$$

where the "centre of the decrease curve" $[M]_c$ denotes the concentration of the third species at which the extrapolated value of k_0 coincides with k_∞. This is illustrated in uig. 1. The dependence of k on [M] is generally speaking complex and the theory of unimolecular reactions has to be applied in its analysis. However, for moderately complex molecules in the region of not unduly high temperatures, an approximate expression is applicable:

$$k = \frac{k_0 k_\infty}{k_0 + k_\infty} F = k_0 \frac{1}{1 + [M]/[M]_c} F = k_\infty \frac{[M]/[M]_c}{1 + [M]/[M]_c} F,$$

where the first terms represent the Lindeman–Hinshelwood equation and the additional expanding multiplier F at not unduly high temperatures is specified[35–37] by

$$\lg F \simeq \frac{\lg F_c}{1 + [\lg([M]/[M]_c)]^2}.$$

Thus, three quantities—k_0, k_∞, and F_c together with

$$[M]_c = \frac{k_\infty}{k_0/[M]}$$

characterise the decrease curves for the purpose under consideration. It is also possible to employ the quantities k_∞, $[M]_c$, and F_c or k_0, $[M]_c$, and F_c. The temperature variation of F_c, which is significant in certain cases, can be estimated by Troe's method[35–37]. The results are usually represented by the approximate equation

$$F_c = (1-a)\exp(-T/T^{***}) + a\exp(-T/T^{*}) + \exp(-T^{**}/T).$$

The first two terms are significant under atmospheric conditions, while the third term begins to contribute in most cases at much higher temperatures. In the first reviews, it was assumed for simplicity that $a = 1$ and that $T_c^{**} \simeq 4T^{*}$. If the values of F_c are known for only one temperature, then the approach remains the same. The term $\exp(-T^{**}/T)$ is frequently negligible at temperatures below 300 K. However, for a more detailed consideration, it is necessary to determine a, T^{***}, T^{*}, and T^{**}. Theoretical predictions[35–37] have been made with the aid of rigorous models of the RRKM type taking into account the influence of weak collisions. For reactions which are significant in the atmosphere, systematic calculations of this type have been published by Patrick and Golden[38]. The question whether these calculations are applicable to barrier-free radical recombination reactions, where rotation effects are important, remains open. The changes in F_c may require changes in the limiting quantities k_0 and k_∞. For the purposes of the present review, this is insignificant in most cases if the recommended values of k_0 and k_∞ agree with the recommended F_c.

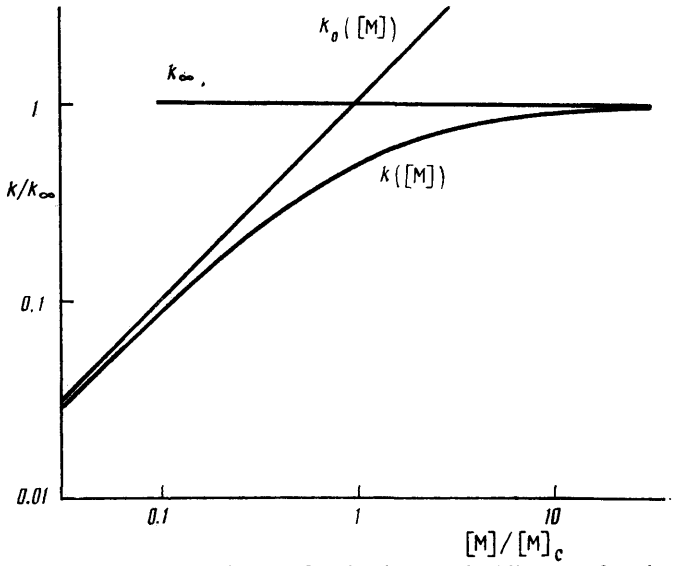


Figure 1. The reduced curve for the decrease in k/k_∞ as a function of $[M]/[M]_c$.

The dependence of k_0 and k_∞ on the temperature T has the form of a power function: $K \propto T^{-n}$ (except in cases with an appreciable energy barrier). This form of the temperature variation has therefore been used because it frequently yields a better agreement with experimental data over a wide temperature range than the Arrhenius law. The dependence of k_0 on the nature of the third species is usually reflected in the relative efficiencies of M_1 and M_2:

$$\{k_0(M_1)/[M_1]\} : \{k_0(M_2)/[M_2]\}.$$

Several thermal dissociation reactions of interest have been examined similarly to recombination reactions with pseudo-first order constants $k(M)$. The rate constants, expressed in s^{-1}, are designated in the Tables by the symbols k_0/s^{-1} and k_∞/s^{-1}. The multiplier F_c has the same significance in recombination and dissociation reactions.

Table 2. Compilation of data for reactions and the recommended rate constants.

Reaction	k_{298}, $cm^3\ s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3\ s^{-1}$	Temperatures range, K	$\Delta (E/R)$, K
		O_x reactions			
$O+O_2+M \rightarrow O_3+M$	$6.2\cdot10^{-34}$ $[O_2]$ (k_0)	±0.1	$6.2\cdot10^{-34}(T/300)^{-2}[O_2]$	200—300	$\Delta n=\pm0.5$
	$5.7\cdot10^{-33}$ $[N_2]$ (k_0)	±0.1	$5.7\cdot10^{-34}(T/300)^{-2.8}[N_2]$	200—300	$\Delta n=\pm0.5$
	$2.8\cdot10^{-12}$ (k_∞)	±0.2	$2.8\cdot10^{-12}$	200—300	$\Delta n=\pm0.5$
	$F_c=0{,}65$	$\Delta F_c=\pm0{,}1$	$F_c=\exp(-T/696)$	200—300	—
$O+O_2 \rightarrow O_3^*$	see Ref.9				
$O_3^*+M \rightarrow O_3+M$	see Ref.9				
$O+O_3 \rightarrow 2O_2$	$8.0\cdot10^{-15}$	±0.08	$8.0\cdot10^{-12}\exp(-2060/T)$	220—400	±200
$O+O_3 \rightarrow$ products	$1.5\cdot10^{-11}$	±0.5	—	—	—
$O(^1D)+O_2 \rightarrow O(^3P)+O_2$	$4.0\cdot10^{-11}$	±0.1	$3.2\cdot10^{-11}\exp(+67/T)$	200—350	±100
$O(^1D)+O_3 \rightarrow O_2+2O(^3P)$	$1.2\cdot10^{-10}$	±0.1	$1.2\cdot10^{-10}$	100—400	±100
$\rightarrow 2O_2(^3\Sigma_g^-)$	$1.2\cdot10^{-10}$	±0.1	$1.2\cdot10^{-10}$	100—400	±100
$O_2^*+O_3 \rightarrow$	see Ref.9				
$O_2(^1\Delta g)+M \rightarrow O_2(^3\Sigma_g^-)+M$	$1.6\cdot10^{-18}$ $(M=O_2)$	±0.2	$3.0\cdot10^{-18}\exp(-200/T)$	100—450	±200
	$\leqslant1.4\cdot10^{-19}$ $(M=N_2)$	—	—	—	—
	$5\cdot10^{-18}$ $(M=H_2O)$	±0.3	—	—	—
	$\leqslant2\cdot10^{-20}$ $(M=CO_2)$	—	—	—	—
$O_2(^1\Sigma_g^+)+M \rightarrow O_2(^3\Sigma_g^-)+M$	$8.0\cdot10^{-14}$ $(M=O)$	±0.3	—	—	—
	$4.0\cdot10^{-17}$ $(M=O_2)$	±0.3	—	—	—
	$2.0\cdot10^{-15}$ $(M=N_2)$	±0.1	$2.0\cdot10^{-15}$	200—300	±200
	$4.0\cdot10^{-12}$ $(M=H_2O)$	±0.3	—	—	—
	$4.1\cdot10^{-13}$ $(M=CO_2)$	±0.1	$4.1\cdot10^{-13}$	245—350	±200
$O_2(^1\Sigma_g^+)+O_3 \rightarrow$ products	$2.2\cdot10^{-11}$ —	±0.06	$2.2\cdot10^{-11}$	295—360	±300
$O_3(^1\Sigma_g^+)+O_2 \rightarrow O_2(^3\Sigma_g^-)+O_2$	see Ref.9				
$O_2+h\nu \rightarrow$ products	see Ref.9				
$O_3+h\nu \rightarrow$ products	see Ref.9				
		HO_x reactions			
$H+HO_2 \rightarrow H_2+O_2$	$5.6\cdot10^{-12}$ —	±0.5	$5.6\cdot10^{-12}$	245—300	±200
$\rightarrow 2HO$	$7.2\cdot10^{-11}$ —	±0.1	$7.2\cdot10^{-11}$	245—300	±200
$\rightarrow H_2O+O$	$2.4\cdot10^{-12}$ —	±0.5	$2.4\cdot10^{-12}$	245—300	±200
$H+O_2+M \rightarrow HO_2+M$	$5.9\cdot10^{-32}$ $[O_2]$ (k_0)	±0.1	$5.9\cdot10^{-32}(T/300)^{-1.0}[O_2]$	200—300	$\Delta n=\pm0.6$
	$5.9\cdot10^{-32}$ $[N_2]$ (k_0)	±0.1	$5.9\cdot10^{-32}(T/300)^{-1.0}[N_2]$	200—300	$\Delta n=\pm0.6$
	$7.5\cdot10^{-11}$ (k_∞)	±0.2	$7.5\cdot10^{-11}(T/300)^{+0.6}$	200—300	$\Delta n=\pm0.6$
	$F_c=0{,}55$	$\Delta F_c=\pm0{,}15$	$F_c=\exp(-T/502)$	200—300	—
$H+O_3 \rightarrow HO+O_2$	$2.8\cdot10^{-11}$	±0.2	$1.4\cdot10^{-10}\exp(-480/T)$	220—360	±100
$H+O_2 \rightarrow HO^*+O_2$	see Ref.9				
$O+H_2 \rightarrow HO+H$	$9\cdot10^{-18}$	±0.2	—	—	—
$O+HO \rightarrow O_2+H$	$3.3\cdot10^{-11}$	±0.1	$2.3\cdot10^{-11}\exp(+110/T)$	220—500	±100
$O+HO_2 \rightarrow HO+O_2$	$5.7\cdot10^{-11}$	±0.08	$2.9\cdot10^{-11}\exp(+200/T)$	200—400	±100
$O+H_2O_2 \rightarrow HO+HO_2$	$1.7\cdot10^{-15}$	±0.3	$1.4\cdot10^{-12}\exp(-2000/T)$	250—390	±1000
$O(^1D)+H_2 \rightarrow HO+H$	$1.1\cdot10^{-10}$	±0.1	$1.1\cdot10^{-10}$	200—350	±100
$O(^1D)+H_2O \rightarrow 2HO$	$2.3\cdot10^{-10}$	±0.1	$2.3\cdot10^{-10}$	200—350	±100
$HO+H_2 \rightarrow H_2O+H$	$6.7\cdot10^{-15}$	±0.1	$7.7\cdot10^{-12}\exp(-2100/T)$	200—450	±200
$HO+H_2(v=1)=H_2O+H$	$8.7\cdot10^{-13}$	±0.3	—	—	—
$HO+HO \rightarrow H_2O+O$	$1.8\cdot10^{-12}$	±0.15	—	—	—
$HO+HO+M \rightarrow H_2O_2+M$	$6.9\cdot10^{-31}$ $[O_2]$ (k_0)	±0.5	$6.9\cdot10^{-31}(T/300)^{-0.8}[O_2]$	200—300	$\Delta n=^{+2}_{-0.8}$
	$6.9\cdot10^{-31}$ $[N_2]$ (k_0)	±0.5	$6.9\cdot10^{-31}(T/300)^{-0.8}[N_2]$	200—300	$\Delta n=^{+2}_{-0.8}$
	$3.0\cdot10^{-11}$ (k_∞)	±0.5	$3.0\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0{,}72$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/913)$	200—300	—
$HO+HO_2 \rightarrow H_2O+O_2$	$1.1\cdot10^{-10}$	±0.1	$4.8\cdot10^{-11}\exp(+250/T)$	250—400	±200
$HO+H_2O_2 \rightarrow H_2O+HO_2$	$1.7\cdot10^{-12}$	±0.1	$2.9\cdot10^{-12}\exp(-160/T)$	240—460	±100
$HO+O_3 \rightarrow HO_2+O_2$	$6.7\cdot10^{-14}$	±0.15	$1.9\cdot10^{-12}\exp(-1000/T)$	220—450	±300
$HO^*+M \rightarrow HO+M$	see Ref.9				
$HO^*+O_3 \rightarrow$ products	see Ref.9				
$HO_2+HO_2 \rightarrow H_2O_2+O_2$	$1.6\cdot10^{-12}$	±0.15	$2.2\cdot10^{-13}\exp(+600/T)$	230—420	±200
$HO_2+HO_2+M \rightarrow H_2O_2+O_2+M$	$4.5\cdot19^{-32}$ $[O_2]$	±0.15	—	—	—
	$5.2\cdot10^{-32}$ $[N_2]$	±0.15	$1.9\cdot10^{-33}\exp(+980/T)$ $[N_2]$	230—420	±300
	influence of H_2O, see Ref.9				
$HO_2+O_3 \rightarrow HO+2O_2$	$2.0\cdot10^{-15}$	±0.2	$1.4\cdot10^{-14}\exp(-600/T)$	250—350	$+500$ -100
$H_2O+h\nu \rightarrow HO+H$	see Ref.9				
$H_2O_2+h\nu \rightarrow 2HO$	see Ref.9				

Table 2 (cont'd.)

Reaction	k_{298}, cm^3 s^{-1}	$\Delta \lg k_{298}$	Temperature dependence of K, cm^3 s^{-1}	Temperatures range, K	$\Delta (E/R)$, K
		NO_x reactions			
$O+NO+M \rightarrow NO_2+M$	$8.6\cdot10^{-32}$ [O_2] (k_0)	±0.2	$8.6\cdot11^{-32}(T/300)^{-1.6}$ [O_2]	200—300	$\Delta n = \pm0.5$
	$1.0\cdot10^{-31}$ [N_2] (k_0)	±0.1	$1.0\cdot10^{-31}(T/300)^{-1.6}$ [N_2]	200—300	$\Delta n = \pm0.5$
	$3.0\cdot10^{-11}$ (k_∞)	±0.2	$3.0\cdot10^{-11}(T/300)^{+0,3}$	300—1500	$\Delta n = \pm0.5$
	$F_c = 0.85$	$\Delta F_c = \pm0.1$	$F_c = \exp(-T/1850)$	200—300	—
$O+NO_2 \rightarrow O_2+NO$	$9.7\cdot10^{-12}$	±0.06	$6.5\cdot10^{-12}\exp(+120/T)$	230—350	±120
$O+NO_2+M \rightarrow NO_3+M$	$9\cdot10^{-32}$ [O_2] (k_0)	±0.3	$9\cdot10^{-32}(T/300)^{-2.0}$ [O_2]	200—400	$\Delta n = \pm1.0$
	$9\cdot10^{-32}$ [N_2] (k_0)	±0.1	$9\cdot10^{-32}(T/300)^{-2.0}$ [N_2]	200—400	$\Delta n = \pm1.0$
	$2.2\cdot10^{-11}$ (k_∞)	±0.1	$2.2\cdot10^{-11}$	200—400	$\Delta n = \pm0.5$
	$F_c = 0,8$	$\Delta F_c = \pm0.1$	$F_c = \exp(-T/1300)$	200—400	—
$O+NO_3 \rightarrow O_2+NO_2$	$1\cdot10^{-11}$	±0.5	—	—	—
$O+N_2O_5 \rightarrow$ products	$\leqslant3\cdot10^{-16}$	—	$\leqslant3\cdot10^{-16}$	220—300	—
$O(^1D)+N_2 \rightarrow O(^3P)+N_2$	$2.6\cdot10^{-11}$	±0.1	$1.8\cdot10^{-11}\exp(+107/T)$	200—350	±100
$O(^1D)+N_2O \rightarrow N_2+O_2$	$4.4\cdot10^{-11}$	±0.15	$4.4\cdot10^{-11}$	200—350	±100
$\rightarrow 2NO$	$7.2\cdot10^{-11}$	±0.15	$7.2\cdot10^{-11}$	200—350	±100
$N+HO \rightarrow NO+H$	$4.9\cdot10^{-11}$	±0.15	$3.8\cdot10^{-11}\exp(+85/T)$	250—500	±100
$N+O_2 \rightarrow NO+O$	$8.9\cdot10^{-17}$	±0.1	$4.4\cdot10^{-12}\exp(-3220/T)$	280—333	±350
$N+O_2(^1\Delta_g) \rightarrow NO+O$	$\leqslant1\cdot10^{-16}$	—	$\leqslant1\cdot10^{-16}$	200—300	—
$N+O_3 \rightarrow NO+O_2$	$1\cdot10^{-16}$	±0.3	—	—	—
$N+NO \rightarrow N_2+O$	$3.1\cdot10^{-11}$	±0.15	$3.1\cdot10^{-11}$	200—400	±100
$N+NO_2 \rightarrow N_2O+O$	$3.0\cdot10^{-12}$	±0.2	—	—	—
$HO+NH_3 \rightarrow H_2O+NH_2$	$1.6\cdot10^{-13}$	±0.15	$3.5\cdot10^{-12}\exp(-925/T)$	230—450	±200
$HO+HONO \rightarrow H_2O+NO_2$	$4.9\cdot10^{-12}$	±0.3	$1.8\cdot10^{-11}\exp(-390/T)$	280—340	±400
$HO+HONO_2 \rightarrow H_2O+NO_3$	$1.5\cdot10^{-13}$ (1 atm)	±0.1	see Ref.9		
$HO+HO_2NO_2 \rightarrow$ products	$5.0\cdot10^{-12}$	±0.2	$1.5\cdot10^{-12}\exp(+360/T)$	240—340	$+300$ -600
$HO+NO+M \rightarrow HONO+M$	$7.4\cdot10^{-31}$ [O_2] (k_0)	±0.2	$7.4\cdot10^{-31}(T/300)^{-2.4}$[$O_2$]	200—440	$\Delta n = \pm1.0$
	$7.4\cdot10^{-31}$ [N_2] (k_0)	±0.1	$7.4\cdot10^{-31}(T/300)^{-2.4}$[$N_2$]	200—440	$\Delta n = \pm0.5$
	$1.0\cdot10^{-11}$ (k_∞)	±0.2	$1.0\cdot10^{-11}$	200—400	$\Delta n = \pm0.5$
	$F_c = 0,8$	$\Delta F_c = \pm0.1$	$F_c = \exp(-T/1300)$	200—400	—
$HO+NO_2+M \rightarrow HONO_2+M$	$2.2\cdot10^{-30}$ [O_2] (k_0)	±0.1	$2.2\cdot10^{-30}(T/300)^{-2.9}$[$O_2$]	200—300	$\Delta n = \pm0.5$
	$2.6\cdot10^{-30}$ [N_2] (k_0)	±0.1	$2.6\cdot10^{-30}(T/300)^{-2.9}$[$N_2$]	200—300	$\Delta n = \pm0.5$
	$5.2\cdot10^{-11}$ (k_∞)	±0.2	$5.2\cdot10^{-11}$	200—300	$\Delta n = \pm0.5$
	$F_c = 0.43$	$\Delta F_c = \pm0.1$	$F_c = \exp(-T/353)$	200—300	—
$HO+NO_3 \rightarrow HO_2+NO_2$	$2.3\cdot10^{-11}$	±0.2	—	—	—
$HO_2+NO \rightarrow HO+NO_2$	$8.3\cdot10^{-12}$	±0.1	$3.7\cdot10^{-12}\exp(+240/T)$	230—500	±100
$HO_2+NO_2+M \rightarrow HO_2NO_2+M$	$1.5\cdot10^{-31}$ [O_2] (k_0)	±0.1	$1.5\cdot10^{-31}(T/300)^{-3/2}$[$O_2$]	220—360	$\Delta n = \pm1$
	$1.8\cdot10^{-31}$ [N_2] (k_0)	±0.1	$1.8\cdot10^{-31}(T/300)^{-3/2}$[$N_2$]	220—360	$\Delta n = \pm1$
	$4.7\cdot10^{-12}$ (k_∞)	±0.1	$4.7\cdot10^{-12}$	200—300	$\Delta n = \pm1$
	$F_c = 0.6$	$\Delta F_c = \pm0.1$	see Ref.9		
$HO_2NO_2+M \rightarrow HO_2+NO_2+M$	$9.3\cdot10^{-21}$ [O_2] (k_0/s^{-1})	±0.3	$3.6\cdot10^{-6}\exp(-10\,000/T)$[$O_2$] c^{-1}	260—300	±500
	$1.3\cdot10^{-20}$ [N_2] (k_0/s^{-1})	±0.3	$5\cdot10^{-6}\exp(-10\,000/T)$[$N_2$] c^{-1}	260—300	±500
	0.23 (k_∞/c^{-1})	±0.6	$3.4\cdot10^{14}\exp(-10420/T)$ c^{-1}	250—300	±500
	$F_c = 0,6$	$\Delta F_c = \pm0.1$	—	—	—
$HO_2+NO_3 \rightarrow O_2+NONO_2$ / $HO+NO_2+O_2$	$4.3\cdot10^{-12}$	±0.2	—	—	—
$NH_2+HO \rightarrow$ products	no recommended value see Ref.9				
$NH_2+HO_2 \rightarrow$ products	$3.4\cdot10^{-11}$	±0.4	—	—	—
$NH_2+O_2 \rightarrow$ products	$<3\cdot10^{-18}$				
$NH_2+O_3 \rightarrow$ products	$1.7\cdot10^{-13}$	±0.5	$4.9\cdot10^{-12}\exp(-1000/T)$	250—380	±500
$NH_2+NO \rightarrow$ products	$1.6\cdot10^{-11}$	±0.3	$1.6\cdot10^{-11}(T/298)^{-1.5}$	210—500	$\Delta n = \pm0.5$
$NH_2+NO_2 \rightarrow$ products	$1.9\cdot10^{-11}$	±0.3	$1.9\cdot10^{-11}(T/298)^{-2.2}$	250—500	$\Delta n = \pm1.5$
$2NO+O_2 \rightarrow 2NO_2$	$2.0\cdot10^{-38}$	±0.1	$3.3\cdot10^{-39}\exp(+530/T)$	273—600	±400
$NO+O_3 \rightarrow NO_2+O_2$	$1.8\cdot10^{-14}$	±0.08	$1.8\cdot10^{-12}\exp(-1370/T)$	195—304	±200
$NO+NO_3 \rightarrow 2NO_2$	$2.7\cdot10^{-11}$	±0.12	$1.6\cdot10^{-11}\exp(+150/T)$	200—300	±100
$NO_2+O_3 \rightarrow NO_3+O_2$	$3.2\cdot10^{-17}$	±0.06	$1.2\cdot10^{-13}\exp(-2450/T)$	230—360	±150
$NO_2+NO_3+M \rightarrow N_2O_5+M$	$2.7\cdot10^{-30}$ [N_2] (k_0)	±0.1	$2.7\cdot10^{-30}(T/300)^{-3.4}$[$N_2$]	200—300	$\Delta n = \pm0.5$
	$2.0\cdot10^{-12}$ (k_∞)	±0.1	$2.0\cdot10^{-12}(T/300)^{+0.2}$	200—500	$\Delta n = \pm0.6$
	$F_c = 0.34$				
$N_2O_5+M \rightarrow NO_2+NO_3+M$	$1.6\cdot10^{-19}$ [N_2] (k_0/s^{-1})	±0.2	$2.2\cdot10^{-3}(T/300)^{-4.4}\exp(-11080/T)$. [$N_2$] s^{-1}	200—300	±500
	$6.9\cdot10^{-2}$ (k_∞/s^{-1})	±0.3	$9.7\cdot10^{14}(T/300)^{+0.1}\exp(-11080/T)$ c^{-1}	200—300	±500
	$F_c = 0.34$	—	—	—	—

Table 2 (cont'd.)

Reaction	k_{298}, $cm^3\ s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3\ s^{-1}$	Temperatures range, K	$\Delta (E/R)$, K
		NO_x reactions			
$N_2O_5 \rightleftarrows NO_2+NO_3$	see Ref.9				
$N_2O_5+H_2O \rightarrow 2HONO_2$	$<2\cdot10^{-21}$	—	—	—	—
$HONO+h\nu \rightarrow$ products	see Ref.9				
$HONO_2+h\nu \rightarrow$ products	see Ref.9				
$HO_2NO_2+h\nu \rightarrow$ products	see Ref.9				
$NO+h\nu \rightarrow$ products	see Ref.9				
$NO_2+h\nu \rightarrow$ products	see Ref.9				
$NO_3+h\nu \rightarrow$ products	see Ref.9				
$N_2O+h\nu \rightarrow$ products	see Ref.9				
$N_2O_5+h\nu \rightarrow$ products	see Ref.9				
		Organic reactions			
$O+CH_3 \rightarrow HCHO+H$	$1.4\cdot10^{-10}$	±0.1	$1.4\cdot10^{-10}$	200—900	±100
$O+CN \rightarrow CO+N(^2D)$	$1.4\cdot10^{-11}$	±0.2	—	—	—
$\rightarrow CO+N(^4S)$	$3.4\cdot10^{-12}$	±0.2	—	—	—
$O(^1D)+CH_4 \rightarrow HO+CH_3$	$1.4\cdot10^{-10}$	±0.1	$1.4\cdot10^{-10}$	200—300	±100
$\rightarrow HCHO+H_2$	$1.5\cdot10^{-11}$	±0.1	$1.5\cdot10^{-11}$	200—300	±100
$HO+CH_4 \rightarrow H_2O+CH_3$	$8.3\cdot10^{-15}$	±0.1	$3.7\cdot10^{-12}\exp(-1820/T)$	240—300	±100
$HO+C_2H_2+M \rightarrow C_2H_2OH+M$	$5\cdot10^{-30}\ [N_2]\ (k_0)$	±0.1	$5\cdot10^{-30}\ [N_2]$	220—300	$\Delta n=\pm1$
	$8.3\cdot10^{-13}\ (k_\infty)$	±0.1	$8.3\cdot10^{-13}\ (T/300)^{+2}$	220—300	$\Delta n=\pm1$
	$F_c=0,6$	$\Delta F_c=\pm0.2$	—	—	—
$HO+C_2H_4+M \rightarrow C_2H_4OH+M$	$9.5\cdot10^{-29}\ [O_2]\ (k_0)$	±0.3	$9.5\cdot10^{-29}\ (T/300)^{-3.1}[O_2]$	200—300	$\Delta n=\pm2$
	$9.5\cdot10^{-29}\ [N_2]\ (k_0)$	±0.3	$9.5\cdot10^{-29}\ (T/300)^{-3.1}[N_2]$	200—300	$\Delta n=\pm2$
	$9\cdot10^{-12}\ (k_\infty)$	±0.3	$9\cdot10^{-12}$	200—300	$\Delta n=\pm1$
	$F_c=0.7$	$\Delta F_c=0.2$	$F_c=\exp(-T/840)$	200—300	—
$HO+C_2H_6 \rightarrow H_2O+C_2H_5$	$2.7\cdot10^{-13}$	±0.1	$7.4\cdot10^{-12}\exp(-990/T)$	230—300	±100
$HO+C_3H_6+M \rightarrow C_3H_6OH+M$	$8\cdot10^{-27}\ [O_2]\ (k_0)$	±1	$8\cdot10^{-27}(T/300)^{-3.5}[O_2]$	200—300	$\Delta n=\pm1$
	$8\cdot10^{-27}\ [N_2]\ (k_0)$	±1	$8\cdot10^{-27}\ (T/300)^{-3.5}[N_2]$	200—300	$\Delta n=\pm1$
	$3.0\cdot10^{-11}\ (k_\infty)$	±0.1	$3.0\cdot10^{-11}$	200—300	$\Delta n=\pm1$
	$F_c=0.5$	$\Delta F_c=\pm0.2$	$F_c=\exp(-T/433)$	—	—
$HO+C_3H_8 \rightarrow H_2O+C_3H_7$	$1.1\cdot10^{-12}$	±0.15	$8.6\cdot10^{-12}\ (-610/T)$	~300	±200
$HO+CO \rightarrow H+CO_2$	$(1.5.10^{-13}).[1+0.6(P/atm)]$ (0—760 mmHg, air)	±0.1	$(1.5.10^{-13})[1+0.6(P/atm)]$ (0—760 mmHg, air)	200—300	±300
$HO+HCHO \rightarrow H_2O+HCO$	$1.1\cdot10^{-11}$	±0.1	$1.6\cdot10^{-11}\exp(-110/T)$	230—580	±150
$HO+CH_3CHO \rightarrow H_2O+CH_3CO$	$1.6\cdot10^{-11}$	±0.1	$5.6\cdot10^{-12}\exp(+310/T)$	240—530	±200
$HO+C_2H_5CHO \rightarrow$ products	$2.0\cdot10^{-11}$	±0.15	—	—	—
$HO+(CHO)_2 \rightarrow$ products	$1.1\cdot10^{-11}$	±0.3	—	—	—
$HO+HOCH_2CHO \rightarrow H_2O+HOCH_2CO$	$8.0\cdot10^{-12}$	±0.3	—	—	—
$\rightarrow H_2O+HOCHCHO$	$2.0\cdot10^{-12}$	±0.3	—	—	—
$HO+CH_3COCHO \rightarrow H_2O+CH_3COCO$	$1.7\cdot10^{-11}$	±0.3	—	—	—
$HO+CH_3COCH_3 \rightarrow H_2O+CH_2COCH_3$	$2.3\cdot10^{-13}$	±0.2	$1.7\cdot10^{-12}\exp(-600/T)$	240—440	±300
$HO+CH_3OH \rightarrow H_2O+CH_2OH$	$9.0\cdot10^{-13}$	±0.2	$9.1\cdot10^{-12}\exp(-690/T)$	240—1000	±250
$\rightarrow H_2O+CH_3O$					
$HO+C_2H_5OH \rightarrow$ products	$3.4\cdot10^{-12}$	±0.2	$9.3\cdot10^{-12}\exp(-300/T)$	250—450	±200
$HO+n\text{-}C_3H_7OH \rightarrow$ products	$5.3\cdot10^{-12}$	±0.2			
$HO+iso\text{-}C_3H_7OH \rightarrow$ products	$5.6\cdot10^{-12}$	±0.2	$5.6\cdot10^{-12}$		
$HO+CH_3OOH \rightarrow H_2O+CH_2OOH$	$4.4\cdot10^{-12}$	±0.3	—	240—440	±200
$\rightarrow H_2O+CH_3OO$	$6.6\cdot10^{-12}$	±0.3	—	—	—
$HO+HCOOH \rightarrow$ products	$4.8\cdot10^{-13}$	±0.2	$4.8\cdot10^{-13}$	—	—
$HO+CH_3COOH \rightarrow$ products	$7.4\cdot10^{-13}$	±0.3	$1.3\cdot10^{-12}\exp(-170/T)$	290—430	±150
$HO+CH_3CO_3NO_2 \rightarrow$ products	$1.4\cdot10^{-13}$	±0.2	$1.2\cdot10^{-12}\exp(-650/T)$	290—440	±300
$HO+HCN \rightarrow$ products	3.10^{-14} (1 atm)	±0.5	$1.2.10^{-13}\exp(-400/T)$(1 atm)	270—300	±400
$HO+CH_3CN \rightarrow$ products	$2.0\cdot10^{-14}$	±0.2	$6.3\cdot10^{-13}\exp(-1030/T)$	296—433	±300
$HO_2+CH_3O_2 \rightarrow O_2+CH_3O_2H$	$4.9\cdot10^{-12}$	±0.3	$1.7\cdot10^{-13}\exp(+1000/T)$	250—360	±250
$HO_2+C_2H_5O_2 \rightarrow O_2+C_2H_5O_2H$	$5.8\cdot10^{-12}$	±0.2	$6.5\cdot10^{-13}\exp(+650/T)$	250—380	±500
$HO_2+HCHO \rightarrow HOCH_2OO$	$7.9\cdot10^{-14}$	±0.2	$9.7\cdot10^{-15}\exp(+625/T)$	240—380	±200
$HOCH_2OO \rightarrow HO_2+HCHO$	$1.5\cdot10^{2}\ c^{-1}$	±0.2	$2.4\cdot10^{12}\exp(-7000/T)$	220—420	±600
$NO_3+C_2H_2 \rightarrow$ products	$<1\cdot10^{-16}$	—	—	—	—
$NO_3+C_2H_4 \rightarrow$ products	$2.1\cdot10^{-16}$	±0.3	—	—	—
$NO_3+C_3H_6 \rightarrow$ products	$9.4\cdot10^{-15}$	±0.2	—	—	—
$NO_3+HCHO \rightarrow HNO_3+HCO$	$6\cdot10^{-16}$	±0.3	—	—	—
$NO_3+CH_3CHO \rightarrow HNO_3+CH_3CO$	$2.7\cdot10^{-15}$	±0.2	$1.4\cdot10^{-12}\exp(-1860/T)$	260—370	±1000
$NO_3+CH_3OH \rightarrow$ products	$<1\cdot10^{-15}$	—	—	—	—
$NO_3+C_2H_5OH \rightarrow$ products	$<2\cdot10^{-15}$	—	—	—	—
$NO_3+iso\text{-}C_3H_7OH \rightarrow$ products	$<5\cdot10^{-15}$	—	—	—	—
$CH_3+O_2+M \rightarrow CH_3O_2+M$	$8\cdot10^{-31}\ [N_2]\ (k_0)$	±0.2	$8\cdot10^{-31}\ (T/300)^{-3.3}[N_2]$	200—600	$\Delta n=\pm1$
	$2.2\cdot10^{-12}\ (k_\infty)$	±0.3	$2.2\cdot10^{-12}\ (T/300)^{1}$	200—400	$\Delta n=\pm1$
	$F_c=0.27$ —	$\Delta F_c=\pm0.1$			
$C_2H_5+O_2 \rightarrow C_2H_4+HO_2$	$<2\cdot10^{-15}$ —	—	$1.4\cdot10^{-12}\exp(-1950/T)$	300—2500	±600

Table 2 (cont'd.)

Reaction	k_{298}, cm^3 s^{-1}	$\Delta \lg k_{298}$	Temperature dependence of K, cm^3 s^{-1}	Temperatures range, K	$\Delta(E/R)$, K
		Organic reactions			
$C_2H_5+O_2+M\rightarrow C_2H_5O_2+M$	$2.0\cdot10^{-28}$ [O_2] (k_0)	±0.3	$2.0\cdot10^{-28}$ $(T/300)^{-3.8}$[O_2]	200—300	$\Delta n=\pm1$
	$2.0\cdot10^{-28}$ [N_2] (k_0)	±0.3	$2.0\cdot10^{-28}$ $(T/300)^{-3.8}$[N_2]	200—300	$\Delta n=\pm1$
	$5.0\cdot10^{-12}$ (k_∞)	±0.3	$5\cdot10^{-12}$	200—300	$\Delta n=\pm1$
	$F_c=0.7$	$\Delta F_c=\pm0.2$	$F_c=\exp(-T/840)$	—	—
n-$C_3H_7+O_2+M\rightarrow n$-$C_3H_7O_2+M	$6\cdot10^{-12}$ (k_∞)	±0.3	$6\cdot10^{-12}$	200—300	$\Delta n=\pm1$
iso-$C_3H_7+O_2+M\rightarrow$ iso-$C_3H_7O_2+M$	$1.5\cdot10^{-11}$ (k_∞)	±0.3	$1.5\cdot10^{-11}$	200—300	$\Delta n=\pm1$
$HCO+O_2\rightarrow CO+HO_2$	$5.6\cdot10^{-12}$	±0.2	$3.5\cdot10^{-12}\exp(+140/T)$	300—500	±150
$CH_3CO+O_2(+M)\rightarrow CH_3CO(+M)$	2.10^{12} (1 – mmHg)	—	—	—	—
	$5\cdot10^{-12}$ (k_∞)	±0.5	$5\cdot10^{-12}$	200—300	$\Delta n=\pm1$
$CH_3O+O_2\rightarrow HCHO+HO_2$	$1.9\cdot10^{-15}$	±0.2	$7.2\cdot10^{-14}\exp(-1080/T)$	298—610	±300
$C_2H_5O+O_2\rightarrow CH_3CHO+HO_2$	$8.0\cdot10^{-15}$	±0.3	—	—	—
n-$C_3H_7O+O_2\rightarrow C_2H_5CHO+HO_2$	$8\cdot10^{-15}$	±0.5	—	—	—
iso-$C_3H_7O+O_2\rightarrow CH_3COCH_3+HO_2$	$8\cdot10^{-15}$	±0.3	$1.5\cdot10^{-14}\exp(-200/T)$	290—390	±200
$CH_2OH+O_2\rightarrow HCHO+HO_2$	$9.8\cdot10^{-12}$	±0.15	—	—	—
$CH_3+O_3\rightarrow$products	$2.5\cdot10^{-12}$	±0.3	$5.1\cdot10^{-12}\exp(-210/T)$	240—400	±200
$CH_3O+NO+M\rightarrow CH_3ONO+M$	$3\cdot10^{-28}$ [He] (k_0)	±0.5	—	—	—
	$6\cdot10^{-28}$ [N_2] (k_0)	±0.5	—	—	—
	$2\cdot10^{-11}$ (k_∞)	±0.3	$2\cdot10^{-11}$	200—400	—
	$F_c=0.6$	—	—	—	—
$RO+NO+M\rightarrow RONO+M$	see Ref.9				
$RO+NO\rightarrow R'O+HNO$	see Ref.9				
$CH_3CH_2O+NO_2+M\rightarrow CH_3ONO_2+M$	$2.6\cdot10^{-29}$ [He] (k_0)	±0.5	$2.6\cdot10^{-29}$ $(T/300-^{-4.5}$[He]	200—400	$\Delta n=\pm2$
	$1.5\cdot10^{-11}$ (k_∞)	±0.3	$1.5\cdot10^{-11}$	300—400	—
	$F_c=0.4$	—	—	—	—
$CH_3O+NO_2\rightarrow HCHO+HONO$	$<3\cdot10^{-13}$	—	$<3\cdot10^{-13}$	200—300	—
$RO+NO_2+M\rightarrow RONO_2+M$	see Ref.9				
$RO+NO_2\rightarrow R'O+HNO$	see Ref.9				
$CH_3O_2+NO\rightarrow CH_3O+NO_2$	$7.6\cdot10^{-12}$	±0.1	$4.2\cdot10^{-12}\exp(+180/T)$	240—360	±180
$C_2H_5O_2+NO\rightarrow C_2H_5O+NO_2$	$8.8\cdot10^{-12}$	±0.3	—	—	—
$C_2H_5O_2+NO(+M)\rightarrow C_2H_5ONO_2(+M)$	$\leqslant1.3\cdot10^{-13}$	—	—	—	—
n-$C_3H_7O_2+NO\rightarrow n$-$C_3H_7O+NO_2$	$8.7\cdot10^{-12}$	±0.3	—	—	—
n-$C_3H_7O_2+NO(+M)\rightarrow n$-$C_3H_7ONO_2(+M)$	$1.8\cdot10^{-13}$	±0.3	—	—	—
iso-$C_3H_7O_2+NO\rightarrow$ iso-$C_3H_7O+NO_2$	$8.5\cdot10^{-12}$	±0.3	—	—	—
iso-$C_3H_7O_2+NO(+M)\rightarrow$ iso-$C_3H_7ONO_2(+M)$	$3.8\cdot10^{-13}$	±0.3	—	—	—
$CH_3CO_3+NO\rightarrow CH_3+CO_2+NO_2$	$1.4\cdot10^{-11}$	±0.7	—	—	—
$CH_3O_2+NO_2+M\rightarrow CH_3O_2NO_2+M$	$2.3\cdot10^{-30}$ [O_2] (k_0)	±0.2	$2.3\cdot10^{-30}$ $(T/300)^{-4.0}$[O_2]	200—300	$\Delta n=\pm2$
	$2.3\cdot10^{-30}$ [N_2] (k_0)	±0.1	$2.3\cdot10^{-30}$ $(T/300)^{-4.0}$[N_2]	200—300	$\Delta n=\pm2$
	$8.0\cdot10^{-12}$ (k_∞)	±0.2	$8\cdot10^{-12}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.4$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/327)$		
$CH_3O_2NO_2+M\rightarrow CH_3O_2+NO_2+M$	$6.8.10^{-19}$ [N_2](k_0/s^{-1})	±0.3	$9.10^{-5}\exp(-9690/T)$[N_2] s^{-1}	250—300	±500
	4.5 (k_∞/s^{-1})	±0.3	$1.1.10^{16}\exp(-10560/T)$ s^{-1}	250—300	±500
	F_c=0.4				
$C_2H_5O_2+NO_2+M\rightarrow C_2H_5O_2NO_2+M$	$5\cdot10^{-12}$ (k_∞)	±0.5	$5\cdot10^{-12}$	200—300	$\Delta n=\pm1$
$C_2H_5O_2NO_2+M\rightarrow C_2H_5O_2+NO_2+M$	no recommended value see Ref.9				
$CH_3CO_3+NO_2+M\rightarrow CH_3CO_3NO_2+M$	$2\cdot10^{-28}$ [N_2] (k_0)	±0.5	—	—	—
	$8.4\cdot10^{-12}$ (k_∞)	±0.3	—	—	—
	F_c=0.27	—	—	—	—
$CH_3CO_3NO_2+M\rightarrow CH_3CO_3+NO_2+M$	$1.5.10^{-20}$ [N_2] (k_0/s^{-1})	±0.5	$6.3.10^{-2}\exp(-12785/T)$ [N_2] s^{-1}	300—320	±1000
	$5.8.10^{-4}$ ($k_{i\infty}$/s^{-1})	±0.3	$2.2.10^{16}\exp(-13435/T)$ s^{-1}	300—320	±500
	F_c=0.27				
$CH_3O_2+CH_3O_2\rightarrow CH_3OH+HCHO+O_2$	$\geqslant2.1\cdot10^{-13}$	±0.3	$1.7\cdot10^{-13}\exp(+220/T)$	200—400	±220
$\rightarrow 2CH_3O+O_2$	$1.3\cdot10^{-13}$	±0.3			
$\rightarrow CH_3OOCH_3+O_2$	$\leqslant3\cdot10^{-14}$	—	—	—	—
$CH_3O_2+CH_3CO_3\rightarrow CH_3O+CH_3CO_2+O_2$	$5.5\cdot10^{-12}$	±0.5	$2.2\cdot10^{-12}\exp(+490/T)$	250—370	±500
$\rightarrow CH_3CO_2H+HCHO+O_2$	$5.5\cdot10^{-12}$	±0.5			
$C_2H_5O_2+C_2H_5O_2\rightarrow C_2H_5OH+CH_3CHO+O_2$	$8.6\cdot10^{-14}$	±0.12	$1.2\cdot10^{-13}\exp(-110/T)$	250—450	$+300$ -100
$\rightarrow 2C_2H_5O+O_2$					
$\rightarrow C_2H_5OOC_2H_5+O_2$					
n-$C_3H_7O_2+n$-$C_3H_7O_2\rightarrow n$-$C_3H_7OH+C_2H_5CHO+O_2$	$3\cdot10^{-13}$	±0.5	—	—	—
n-$C_3H_7O_2+n$-$C_3H_7O_2\rightarrow 2n$-$C_3H_7O+O_2$	$4.4\cdot10^{-16}$	±0.3	$6.0\cdot10^{-14}\exp(-1460/T)$	300—400	±300
iso-$C_3H_7O_2+$ iso-$C_3H_7O_2\rightarrow$ iso-$C_3H_7OH+CH_3COCH_3+O_2$	$5.6\cdot10^{-16}$	±0.3	$3.2\cdot10^{-12}\exp(-2580/T)$	300—400	±300
iso-$C_3H_7O_2+$ iso-$C_3H_7O_2\rightarrow 2$iso-$C_3H_7O+O_2$	$1.6\cdot10^{-11}$	±0.5	$2.8\cdot10^{-12}\exp(+530/T)$	250—370	±500
$CH_3CO_3+CH_3CO_3\rightarrow 2CH_3CO_2+O_2$					
$RCHO+H_2O\rightarrow RCOOH+H_2O$	no recommended value see Ref.9				
$RCHO+NO_2\rightarrow RCHO+NO_3$					
$RCHO+SO_2\rightarrow$products					
$RCHO+HCHO\rightarrow$products					
$CN+O_2\rightarrow$products	$2.1\cdot10^{-11}$	±0.15	$1.1\cdot10^{-11}\exp(+205/T)$	290—760	±200
	$1\cdot10^{-20}$	±1.0			

Table 2 (cont'd.)

Reaction	k_{298}, $cm^3\ s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3\ s^{-1}$	Temperatures range, K	$\Delta (E/R)$, K
		Organic reactions			
$O_3+C_2H_2\rightarrow$products	$1.7\cdot10^{-18}$	±0.1	$1.2\cdot10^{-14}\exp(-2630/T)$	180—360	±100
$O_3+C_2H_4\rightarrow$products	$1.1\cdot10^{-17}$	±0.15	$1.3\cdot10^{-14}\exp(-2105/T)$	250—360	±400
$O_3+C_3H_6\rightarrow$products	see Ref.9				
$HCHO+h\nu\rightarrow$products	see Ref.9				
$CH_3CHO+h\nu\rightarrow$products	see Ref.9				
$C_2H_5CHO+h\nu\rightarrow$products	see Ref.9				
$(CHO)_2+h\nu\rightarrow$products	see Ref.9				
$CH_3COCHO+h\nu\rightarrow$products	see Ref.9				
$CH_3COCH_3+h\nu\rightarrow$products	see Ref.9				
$CH_3OOH+h\nu\rightarrow$products	see Ref.9				
$CH_3O_2NO_2+h\nu\rightarrow$products	see Ref.9				
$CH_3CO_3NO_2+h\nu\rightarrow$products	see Ref.9				
		SO_x reactions			
$O+H_2S\rightarrow HO+HS$	$2.2\cdot10^{-14}$	±0.3	$1.4\cdot10^{-11}\exp(-1920/T)$	290—500	±750
$O+CS\rightarrow CO+S$	$2.1\cdot10^{-11}$	±0.1	$2.7\cdot10^{-10}\exp(-760/T)$	150—300	±250
$O+CH_3SCH_3\rightarrow CH_3SO+CH_3$	$5.0\cdot10^{-11}$	±0.1	$1.3\cdot10^{-11}\exp(+409/T)$	270—560	±100
$O+CS_2\rightarrow SO+CS$	$3.6\cdot10^{-12}$	±0.2	$3.2\cdot10^{-11}\exp(-650/T)$	200—500	±100
$O+CH_3SSCH_3\rightarrow CH_3SO+CH_3S$	$1.3\cdot10^{-10}$	±0.3	$5.5\cdot10^{-11}\exp(+250/T)$	290—570	±100
$O+OCS\rightarrow SO+CO$	$1.4\cdot10^{-14}$	±0.2	$2.6\cdot10^{-11}\exp(-2250/T)$	220—600	±150
$O+SO_2+M\rightarrow SO_3+M$	$1.4\cdot10^{-33}\ [O_2]\ (k_0)$	±0.3	$4.0\cdot10^{-32}\exp(-1000/T)[O_2]$	200—400	$+200$ -100
$O+SO_2+M\rightarrow SO_3+M$	$1.4\cdot10^{-33}\ [N_2]\ (k_0)$	±0.3	$4.0\cdot10^{-32}\exp(-1000/T)[O_2]$	200—400	$+200$ -100
$S+O_2\rightarrow SO+O$	$2.3\cdot10^{-12}$	±0.2	$2.3\cdot10^{-12}$	230—400	±200
$S+O_3\rightarrow SO+O_2$	$1.2\cdot10^{-11}$	±0.3			
$HO+H_2S\rightarrow H_2O+HS$	$4.8\cdot10^{-12}$	±0.08	$6.3\cdot10^{-12}\exp(-80/T)$	200—300	±80
$HO+CH_3SH\rightarrow$products	$3.3\cdot10^{-11}$	±0.1	$9.9\cdot10^{-12}\exp(+356/T)$	240—430	±100
$HO+CH_3SCH_3\rightarrow H_2O+CH_2SCH_3$	$4.4\cdot10^{-12}$	±0.1	$9.6\cdot10^{-12}\exp(-234/T)$	250—400	±300
$\rightarrow CH_3S(OH)CH_3$	$1.7\cdot10^{-12}$ (1 atm, air)	±0.3	см. [9]		
$HO+CS_2\rightarrow$products	$\leqslant7.0\cdot10^{-15}$ ($[O_2]=0$)				
	$2.0\cdot10^{-12}$ (1 atm, air)	±0.3	$8.8\cdot10^{-16}\exp(+2300/T)$	260—300	±500
$HO+CH_3SSCH_3\rightarrow$products	$2.0\cdot10^{-10}$	±0.1	$6.0\cdot10^{-11}\exp(+380/T)$	250—370	±300
$HO+OCS\rightarrow$products	$2.0\cdot10^{-15}$	±0.3	$1.1\cdot10^{-13}\exp(-1200/T)$	250—500	±500
$HO+SO_2+M\rightarrow HOSO_2+M$	$5.0\cdot10^{-31}\ [O_2]\ (k_0)$	±0.3	$5.0\cdot10^{-31}\ (T/300)^{-3,3}[O_2]$	200—300	$\Delta n=\pm0.5$
	$5.0\cdot10^{-31}\ [N_2]\ (k_0)$	±0.3	$5.0\cdot10^{-31}\ (T/300)^{-3,3}[N_2]$	200—300	$\Delta n=\pm0.5$
	$2\cdot10^{-12}\ (k_\infty)$	±0.3	$2\cdot10^{-12}$	200—300	$\Delta n=\pm1$
	$F_c=0.45$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/380)$	200—300	—
$HOSO_2+O_2\rightarrow HO_2+SO_3$	$4.0\cdot10^{-13}$	±0.1	—	—	—
$HO_2+SO_2\rightarrow$products	$\leqslant1\cdot10^{-18}$	—	—	—	—
$NO_3+H_2H_2S\rightarrow$products	$<1\cdot10^{-15}$	—	—	—	—
$NO_3+CS_2\rightarrow$products	$<1\cdot10^{-15}$	—	—	—	—
$NO_3+OCS\rightarrow$products	$<3\cdot10^{-15}$	—	—	—	—
$NO_3+SO_2\rightarrow$products	$<1\cdot10^{-19}$	—	—	—	—
$NO_3+CH_3SH\rightarrow$products	$9.2\cdot10^{-13}$	±0.15	$9.2\cdot10^{-13}$	250—370	±400
$NO_3+CH_3SCH_3\rightarrow$products	$1.0\cdot10^{-12}$	±0.15	$1.9\cdot10^{-13}\exp(+500/T)$	250—380	±300
$NO_3+CH_3SSCH_3\rightarrow$products	$7\cdot10^{-13}$	±0.3	$7\cdot10^{-13}$	300—380	±500
$CH_3O_2+SO_2\rightarrow CH_3O+SO_3$	$<5\cdot10^{-17}$				
$\rightarrow CH_3O_2SO_2$	no recommended value see Ref.9				
$HS+O_2\rightarrow HO+SO$	$\leqslant4\cdot10^{-19}$	—	—	—	—
$HS+O_3\rightarrow HSO+O_2$	$3.6\cdot10^{-12}$	±0.2	—	—	—
$HS+NO+M\rightarrow HSNO+M$	$2.4\cdot10^{-31}\ [N_2]\ (k_0)$	±0.3	$2.4\cdot10^{-31}\ (T/300)^{-2,5}[N_2]$	200—300	$\Delta n=\pm1$
	$2.7\cdot10^{-11}\ (k_\infty)$	±0.5	$2.7\cdot10^{-11}$	200—300	—
	$F_c=0,6$	—	—	—	—
$HS+NO_2\rightarrow HSO+NO$	$5.8\cdot10^{-11}$	±0.3	$2,6\cdot10^{-11}\exp(+240/T)$	220—450	$+200$
$HSO+O_2\rightarrow$products	$\leqslant2\cdot10^{-17}$	—	—	—	—
$HSO+O_3\rightarrow$products	$1.1\cdot10^{-13}$	±0.8	—	—	—
$HSO+NO\rightarrow$products	$\leqslant1\cdot10^{-15}$	—	—	—	—
$HSO+NO_2\rightarrow$products	$9.6\cdot10^{-12}$	±0.3	—	—	—
$HSO_2+O_2\rightarrow$products	$3\cdot10^{-13}$	±0.8	—	—	—
$SO+O_2\rightarrow SO_2+O$	$6.7\cdot10^{-17}$	±0.15	$1.4\cdot10^{-13}\exp(-2275/T)$	230—420	±500
$SO+O_3\rightarrow SO_2+O_2$	$8.9\cdot10^{-14}$	±0.1	$4.5\cdot10^{-12}\exp(-1170/T)$	230—420	±150
$SO+NO_2\rightarrow SO_2+NO$	$1.4\cdot10^{-11}$	±0.1	$1.4\cdot10^{-11}$	210—360	±100
$SO_3+H_2O\rightarrow$products	no recommended value see Ref.9				
$CS+O_2\rightarrow$products	no recommended value see Ref.9				
$O_3+CH_3SCH_3\rightarrow$products	$<1\cdot10^{-18}$	—	—	—	—
$OCS+h\nu\rightarrow$products	see Ref.9				
$CS_2+h\nu\rightarrow$products	see Ref.9				
$CH_3SSCH_3+h\nu\rightarrow$products	see Ref.9				

Table 2 (cont'd.)

Reaction	k_{298}, cm^3 s^{-1}	$\Delta \lg k_{298}$	Temperature dependence of K, cm^3 s^{-1}	Temperatures range, K	$\Delta(E/R)$, K
		FO_x reactions			
$O+FO \rightarrow O_2+F$	$5\cdot10^{-11}$	±0.5	—	—	—
$O+FO_2 \rightarrow O_2+FO$	$5\cdot10^{-11}$	±0.7	—	—	—
$O(^1D)+HF \rightarrow HO+F$	$1\cdot10^{-10}$	±0.5	—	—	—
$O(^1D)+COF_2 \rightarrow CO_2+F_2$	$2.2\cdot10^{-11}$	±0.2	—	—	—
$\rightarrow O(^3P)+COF_2$	$5.2\cdot10^{-11}$	±0.2	—	—	—
$F+H_2 \rightarrow HF+H$	$2.8\cdot10^{-11}$	±0.1	$1.9\cdot10^{-10}\exp(-570/T)$	190—770	±150
$F+H_2O \rightarrow HF+HO$	$1.1\cdot10^{-11}$	±0.5	$4.2\cdot10^{-11}\exp(-400/T)$	240—370	±200
$F+O_2+M \rightarrow FO_2+M$	$4.3\cdot10^{-33}$ [N_2] (k_0)	±0.3	$4.3\cdot10^{-33}(T/300)^{-1.4}$[$N_2$]	200—300	$\Delta n=\pm1$
	$3\cdot10^{-11}$ (k_∞)	±0.5	$3\cdot10^{-11}$	200—300	$\Delta n=\pm1$
	$F_c=0.85$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/1850)$	200—300	—
$FO_2+M \rightarrow F+O_2+M$	**$2.2.10^{-17}$ [N_2] (k_0/s^{-1})**	±0.5	**$6.3.10^{-9}\exp(-5800/T)$ [N_2] s^{-1}**	200—400	±1000
$F+O_3 \rightarrow FO+O_2$	$1.3\cdot10^{-11}$	±0.3	$2.8\cdot10^{-11}\exp(-226/T)$	250—365	±200
$F+NO_2+M \rightarrow FONO+M$	$1.0\cdot10^{-30}$ [O_2] (k_0)	±0.5	$1.0\cdot10^{-30}(T/300)^{-2.0}$[$O_2$]	200—300	$\Delta n=\pm1$
	$1.0\cdot10^{-30}$ [N_2] (k_0)	±0.5	$1.0\cdot10^{-30}(T/300)^{-2.0}$[$N_2$]	200—300	$\Delta n=\pm1$
	$2\cdot10^{-10}$ (k_∞)	±0.8	$2\cdot10^{-10}$	200—300	$\Delta n=\pm1$
	$F_c=0.6$	$\Delta F_c=\pm0.2$	$F_c=\exp(-T/587)$	200—300	
$F+CH_4 \rightarrow HF+CH_3$	$8.0\cdot10^{-11}$	±0.2	$3.0\cdot10^{-10}\exp(-400/T)$	250—450	±200
$HO+CH_3CHF_2 \rightarrow$ products	$3.4\cdot10^{-14}$	±0.2	—	—	—
$HO+CH_2FCF_3 \rightarrow H_2O+CHFCF_3$	$8.4\cdot10^{-15}$	±0.2	$6.6\cdot10^{-13}\exp(-1300/T)$	250—440	±300
$FO+O_3 \rightarrow$ products	**no recommended value see Ref.9**				
$FO+NO \rightarrow F+NO_2$	$2.6\cdot10^{-11}$	±0.3	—	—	—
$FO+NO_2+M \rightarrow FONO_2+M$	$1.6\cdot10^{-31}$ [O_2] (k_0)	±0.7	$1.6\cdot10^{-31}(T/300)^{-3.4}$[$O_2$]	200—300	$\Delta n=\pm1.0$
	$1.6\cdot10^{-31}$ [N_2] (k_0)	±0.7	$1.6\cdot10^{-31}(T/300)^{-3.4}$[$N_2$]	200—300	$\Delta n=\pm1.0$
	$2\cdot10^{-11}$ (k_∞)	±0.5	$2\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.5$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/433)$	200—300	—
$FO+FO \rightarrow$ products	$1.5\cdot10^{-11}$	±0.3	—	—	—
$HF+h\nu \rightarrow$ products	**see Ref.9**				
$FONO_2+h\nu \rightarrow$ products	**see Ref.9**				
$COF_2+h\nu \rightarrow$ products	**see Ref.9**				
		ClO_x reactions			
$O+HCl \rightarrow HO+Cl$	$1.4\cdot10^{-16}$	±0.3	$1.0\cdot10^{-11}\exp(-3340/T)$	293—718	±350
$O+HOCl \rightarrow HO+ClO$	**no recommended value see Ref.9**				
$O+ClO \rightarrow O_2+Cl$	$3.8\cdot10^{-11}$	±0.1	$3.8\cdot10^{-11}$	200—300	±250
$O+OClO \rightarrow O_2+ClO$ / $\rightarrow O+ClOO$	$5\cdot10^{-13}$	±0.5	—	—	—
$O+ClONO_2 \rightarrow$ products	$1.9\cdot10^{-13}$	±0.1	$3.0\cdot10^{-12}\exp(-808/T)$	213—295	±200
$O(^1D)+CF_2Cl_2 \rightarrow$ products	$1.4\cdot10^{-10}$	±0.1	—	—	—
$O(^1D)+CFCl_3 \rightarrow$ products	$2.3\cdot10^{-10}$	±0.1	—	—	—
$O(^1D)+CCl_4 \rightarrow$ products	$3.3\cdot10^{-10}$	±0.1	—	—	—
$Cl+H_2 \rightarrow HCl+H$	$1.6\cdot10^{-14}$	±0.1	$3.7\cdot10^{-11}\exp(-2300/T)$	200—300	±200
$Cl+HO_2 \rightarrow HCl+O_2$	$3.2\cdot10^{-11}$	±0.2	$1.8\cdot10^{-11}\exp(+170/T)$	250—420	±250
$\rightarrow ClO+HO$	$9.1\cdot10^{-12}$	±0.3	$4.1\cdot10^{-11}\exp(-450/T)$	250—420	±250
$Cl+H_2O_2 \rightarrow HCl+HO_2$	$4.3\cdot10^{-13}$	±0.2	$1.1\cdot10^{-11}\exp(-980/T)$	265—424	±500
$Cl+O_2+M \rightarrow ClOO+M$	$1.7\cdot10^{-33}$ [N_2]	±0.3	—	—	—
$ClOO+M \rightarrow Cl+O_2+M$	**$2.5.10^{-13}$ [N_2] (k/s^{-1})**	±0.5	**$1.5.10^{-8}\exp(-3285/T)$ [NH_3] s^{-1}**	200—300	±1250
$Cl+O_3 \rightarrow ClO+O_2$	$1.2\cdot10^{-11}$	±0.06	$2.7\cdot10^{-11}\exp(-257/T)$	205—298	±100
$Cl+HONO_2 \rightarrow HCl+NO_3$	$<2.0\cdot10^{-16}$	—	—	—	—
$Cl+NO_3 \rightarrow ClO+NO_2$	$2.6\cdot10^{-11}$	±0.3	$2.6\cdot10^{-11}$	200—300	±400
$Cl+CH_4 \rightarrow HCl+CH_3$	$1.0\cdot10^{-13}$	±0.1	$9.6\cdot10^{-12}\exp(-1350/T)$	200—300	±250
$Cl+C_2H_6 \rightarrow HCl+C_2H_5$	$5.7\cdot10^{-11}$	±0.06	$7.7\cdot10^{-11}\exp(-90/T)$	220—350	±100
$Cl+C_3H_8 \rightarrow HCl+C_3H_7$	$1.5\cdot10^{-10}$	±0.2	$1.3\cdot10^{-10}\exp(+40/T)$	220—600	±200
$Cl+HCHO \rightarrow HCl+HCO$	$7.3\cdot10^{-11}$	±0.06	$8.2\cdot10^{-11}\exp(-34/T)$	200—500	±100
$Cl+CH_3CHO \rightarrow HCl+CH_3CO$	$7.6\cdot10^{-11}$	±0.3	—	—	—
$Cl+CH_3CN \rightarrow$ products	$\leq2\cdot10^{-15}$	—	—	—	—
$Cl+OClO \rightarrow 2ClO$	$5.8\cdot10^{-11}$	±0.1	$3.4\cdot10^{-11}\exp(+160/T)$	298—450	±200
$Cl+ClONO_2 \rightarrow Cl_2+NO_3$	$1.2\cdot10^{-11}$	±0.12	$6.8\cdot10^{-12}\exp(+160/T)$	219—298	±200
$Cl+CH_3Cl \rightarrow HCl+CH_2Cl$	$4.9\cdot10^{-13}$	±0.1	$3.4\cdot10^{-11}\exp(-1260/T)$	233—350	±200
$Cl+CH_3CCl_3 \rightarrow HCl+CH_2CCl_3$	$<4\cdot10^{-14}$	±0.1	—	—	—
$HO+HCl \rightarrow H_2O+Cl$	$8.1\cdot10^{-13}$	±0.1	$2.4\cdot10^{-12}\exp(-330/T)$	200—300	±150
$HO+HOCl \rightarrow H_2O+ClO$	$5.0\cdot10^{-13}$	±0.5	$3.0\cdot10^{-12}\exp(-500/T)$	200—300	±500
$HO+ClO \rightarrow HO_2+Cl$ / $\rightarrow HCl+O_2$	$1.7\cdot10^{-11}$	±0.2	$1.1\cdot10^{-11}\exp(+120/T)$	200—373	±150
$HO+OClO \rightarrow HOCl+O_2$	$7.0\cdot10^{-12}$	±0.3	$4.5\cdot10^{-13}\exp(+800/T)$	290—480	±200
$HO+ClONO_2 \rightarrow$ products	$3.9\cdot10^{-13}$	±0.2	$1.2\cdot10^{-12}\exp(-330/T)$	246—387	±200
$HO+CH_3Cl \rightarrow H_2O+CH_2Cl$	$4.2\cdot10^{-14}$	±0.1	$1.9\cdot10^{-12}\exp(-1120/T)$	247—350	±200
$HO+CH_2FCl \rightarrow H_2O+CHFCl$	$4.4\cdot10^{-14}$	±0.1	$2.6\cdot10^{-12}\exp(-1210/T)$	245—350	±100
$HO+CHF_2Cl \rightarrow H_2O+CF_2Cl$	$4.7\cdot10^{-15}$	±0.1	$1.1\cdot10^{-12}\exp(-1620/T)$	250—360	±100
$HO+CHFCl_2 \rightarrow H_2O+CFCl_2$	$3.0\cdot10^{-14}$	±0.1	$1.1\cdot10^{-12}\exp(-1070/T)$	240—350	±100

Table 2 (cont'd.)

Reaction	k_{298}, $cm^3\ s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3\ s^{-1}$	Temperatures range, K	$\Delta (E/R)$, K
		ClO_x reactions			
$HO+CH_2Cl_2 \rightarrow H_2O+CHCl_2$	$1.4\cdot10^{-13}$	±0.1	$4.4\cdot10^{-12}\exp(-1030/T)$	240—300	±250
$HO+CHCl_3 \rightarrow H_2O+CCl_3$	$1.0\cdot10^{-13}$	±0.1	$3.3\cdot10^{-12}\exp(-1030/T)$	240—300	±100
$HO+CFCl_3 \rightarrow HOCl+CFCl_2$	$<5\cdot10^{-18}$	—	$<1\cdot10^{-12}\exp(-3650/T)$	250—480	—
$HO+CF_2Cl_2 \rightarrow HOCl+CF_2Cl$	$<7\cdot10^{-18}$	—	$<1\cdot10^{-12}\exp(-3540/T)$	250—478	—
$HO+CCl_4 \rightarrow HOCl+CCl_3$	$<4\cdot10^{-16}$	—	$<1\cdot10^{-12}\exp(-2320/T)$	—	—
$HO+C_2HCl_3 \rightarrow$ products	$2.2\cdot10^{-12}$	±0.1	$5.0\cdot10^{-13}\exp(+445/T)$	230—420	±200
$HO+C_2Cl_4 \rightarrow$ products	$1.7\cdot10^{-13}$	±0.1	$9.4\cdot10^{-12}\exp(-1200/T)$	300—420	±200
$HO+CH_3CF_2Cl \rightarrow H_2O+CH_2CF_2Cl$	$3.6\cdot10^{-15}$	±0.2	$1.6\cdot10^{-12}\exp(-1820/T)$	270—380	±300
$HO+CHFClCF_3 \rightarrow H_2O+CFClCF_3$	$1.0\cdot10^{-14}$	±0.2	$6.4\cdot10^{-13}\exp(-1240/T)$	250—380	±300
$HO+CH_2ClCF_2Cl \rightarrow H_2O+CHClCF_2Cl$	$1.5\cdot10^{-14}$	±0.3	$3.0\cdot10^{-12}\exp(-1580/T)$	250—350	±500
$HO+CHCl_2CF_3 \rightarrow H_2O+CCl_2CF_3$	$3.4\cdot10^{-14}$	±0.2	$1.2\cdot10^{-12}\exp(-1060/T)$	245—375	±300
$HO+CH_3CCl_3 \rightarrow H_2O+CH_2CCl_3$	$1.2\cdot10^{-14}$	±0.15	$5.1\cdot10^{-12}\exp(-1800/T)$	250—460	±200
$NO_3+C_2HCl_3 \rightarrow$ products	$2.9\cdot10^{-16}$	±0.3	—	—	—
$NO_3+C_2Cl_4 \rightarrow$ products	$<1\cdot10^{-16}$	—	—	—	—
$ClO+HO_2 \rightarrow HOCl+O_2$	$5.0\cdot10^{-12}$	±0.15	$4.6\cdot10^{-13}\exp(+710/T)$	200—300	±300
$\rightarrow HCl+O_3$	$\leqslant2\cdot10^{-14}$	—	—	—	
$ClO+O_2(^1\Delta_g) \rightarrow$ sym-ClO_3	$<3.0\cdot10^{-15}$	—	—	—	—
$ClO+NO \rightarrow Cl+NO_2$	$1.7\cdot10^{-11}$	±0.1	$6.2\cdot10^{-12}\exp(+294/T)$	202—415	±100
$ClO+NO_2+M \rightarrow ClONO_2+M$	$1.7\cdot10^{-31}$ [O_2] (k_0)	±0.1	$1.7\cdot10^{-31}\ (T/300)^{-3.4}$[$O_2$]	200—300	$\Delta n=\pm1.0$
	$1.7\cdot10^{-31}$ [N_2] (k_0)	±0.1	$1.7\cdot10^{-31}\ (T/300)^{-3.4}$[$N_2$]	200—300	$\Delta n=\pm1.0$
	$2\cdot10^{-11}$ (k_∞)	±0.3	$2\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.5$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/430)$	—	—
$ClO+NO_3 \rightarrow ClOO+NO_2$ $\rightarrow OClO+NO_2$	$4.0\cdot10^{-13}$	±0.3	—	—	—
$ClO+HCHO \rightarrow$ products	$<10^{-15}$	—	—	—	—
$ClO+ClO \rightarrow ClOO+Cl$	$3.4\cdot10^{-15}$	±0.2	—	—	—
$\rightarrow OClO+Cl$	$1.7\cdot10^{-15}$	±0.2	—	—	—
$\rightarrow Cl_2+O_2$	$4.9\cdot10^{-15}$	±0.2	—	—	—
$ClO+ClO+M \rightarrow Cl_2O_2+M$	$4.0\cdot10^{-32}$ [N_2] (k_0)	±0.2	$4.0\cdot10^{-32}\ (T/300)^{-2.0}$[$N_2$]	200—300	$\Delta n=\pm1.0$
$Cl_2O_2+M \rightarrow ClO+ClO+M$	$6.1\cdot10^{-18}$ [N_2] (k_0/s^{-1})	±0.5	$3.1\cdot10^{-5}\ (T/300)^{-3}\exp(-8720/T)$ [N_2] s^{-1}	230—300	±500
$OClO+NO \rightarrow ClO+NO_2$	$3.4\cdot10^{-13}$	±0.3	—	—	—
$ClONO_2+H_2O \rightarrow HOCl+HONO_2$	$<5.0\cdot10^{-21}$	—	—	—	—
$ClONO_2+HCl \rightarrow Cl_2+HONO_2$	$<2.0\cdot10^{-20}$	—	—	—	—
$CF_3+O_2+M \rightarrow CF_3O_2+M$	$1.9\cdot10^{-29}$ [N_2] (k_0)	±0.2	$1.9\cdot10^{-29}\ (T/300)^{-4.7}$[$N_2$]	200—400	$\Delta n=\pm1$
	$1\cdot10^{-11}$ (k_∞)	±0.2	$1\cdot10^{-11}$	200—400	—
	$F_c=0.4$—0.5	—	—	—	—
$CFCl_2+O_2+M \rightarrow CFCl_2O_2+M$	$5\cdot10^{-30}$ [N_2] (k_0)	±0.4	$5\cdot10^{-30}\ (T/300)^{-4}$[$N_2$]	200—300	$\Delta n=\pm2$
	$6\cdot10^{-12}$ (k_∞)	±0.5	$6\cdot10^{-12}$	200—300	—
	$F_c=0.6$	—	—	—	—
$CCl_3+O_2+M \rightarrow CCl_3O_2+M$	$1.5\cdot10^{-30}$ [N_2] (k_0)	±0.5	$1.5\cdot10^{-30}\ (T/300)^{-4}$[$N_2$]	200—300	$\Delta n=\pm2$
	$5\cdot10^{-12}$ (k_∞)	±0.5	$5\cdot10^{-12}$	200—300	—
	$F_c=0.25$				
$CCl_3O \rightarrow CCl_2O+Cl$	$>1.10^5\ s^{-1}$ (233 K, 7.5 mmHg)	—	—	—	—
$CCl_2FO \rightarrow CClFO+Cl$	$>3.10^4\ s^{-1}$ (253 K, 6.7 mmHg)	—	—	—	—
$CF_3O_2+NO \rightarrow CF_3O+NO_2$	$1.6\cdot10^{-11}$	±0.2	$1.6\cdot10^{-11}\ (T/300)^{-1.2}$	230—430	—
$CF_2ClO_2+NO \rightarrow CF_2ClO+NO_2$	$1.6\cdot10^{-11}$	±0.3	$1.6\cdot10^{-11}\ (T/300)^{-1.5}$	230—430	—
$CFCl_2O_2+NO \rightarrow CFCl_2O+NO_2$	$1.5\cdot10^{-11}$	±0.2	$1.5\cdot10^{-11}\ (T/300)^{-1.3}$	230—430	—
$CCl_3O_2+NO \rightarrow CCl_3O+NO_2$	$1.8\cdot10^{-11}$	±0.2	$1.8\cdot10^{-11}\ (T/300)^{-1.0}$	230—430	—
$CF_3O_2+NO_2+M \rightarrow CF_3O_2NO_2+M$	$2.7\cdot10^{-29}$ [N_2] (k_0)	±0.3	$2.7\cdot10^{-29}\ (T/300)^{-5}$[$N_2$]	200—300	$\Delta n=\pm2$
	$9\cdot10^{-12}$ (k_∞)	±0.5	$9\cdot10^{-12}\ (T/300)^{-0.7}$	200—300	$\Delta n=\pm1$
	$F_c=0.49$		$F_c=\exp(-T/416)$	—	—
$CF_2ClO_2+NO_2+M \rightarrow CF_2ClO_2NO_2+M$	$4.0\cdot10^{-29}$ [N_2] (k_0)	±0.4	$4.0\cdot10^{-29}\ (T/300)^{-5}$[$N_2$]	200—300	$\Delta n=\pm2$
	$1.0\cdot10^{-11}$ (k_∞)	±0.5	$1.0\cdot10^{-11}\ (T/300)^{-0.7}$	200—300	$\Delta n=\pm1$
	$F_c=0.45$	—	$F_c=\exp(-T/373)$	—	—
$CF_2ClO_2NO_2+M \rightarrow CF_2ClO_2+NO_2+M$	$1.5.10^{-17}$ [N_2] (k_0/s^{-1})	±0.3	$5.6.10^{-4}\exp(-9310/T)$ [N_2] s^{-1}	260—290	±1000
	$4.9.10^{-2}$ (k_∞/s^{-1})	±0.3	$1.0.10^{16}\exp(-11880/T)\ s^{-1}$	260—290	±1000
	$F_c=0.4$	—	—	—	—
$CFCl_2O_2+NO_2+M \rightarrow CFCl_2O_2NO_2+M$	$5.5\cdot10^{-29}$ [N_2] (k_0)	±0.3	$5.5\cdot10^{-29}\ (T/300)^{-5}$[$N_2$]	200—300	$\Delta n=\pm1$
	$8.3\cdot10^{-12}$ (k_∞)	±0.3	$8.3\cdot10^{-12}\ (T/300)^{-0.7}$	200—300	$\Delta n=\pm1$
	$F_c=0.42$		$F_c=\exp(-T/342)$	—	—
$CFCl_2O_2NO_2+M \rightarrow CFCl_2O_2+NO_2+M$	$1.2.10^{-18}$ [N_2] (k_0/s^{-1})	±0.3	$3.10^{-3}\exp(-10570/T)$ [N_2] s^{-1}	270—290	±1000
	$7.3.10^{-2}$ (k_∞/s^{-1})	±0.3	$2.1.10^{16}\exp(-11980/T)\ s^{-1}$	270—290	±1000
	$F_c=0.4$		$F_c=\exp(-T/342)$	—	—
$CCl_3O_2+NO_2+M \rightarrow CCl_3O_2NO_2+M$	$9.2\cdot10^{-29}$ [N_2] (k_0)	±0.3	$9.2\cdot10^{-29}\ (T/300)^{-6}$[$N_2$]	200—300	$\Delta n=\pm2$
	$1.5\cdot10^{-11}$ (k_∞)	±0.3	$1.5\cdot10^{-11}\ (T/300)^{-0.3}$	200—300	$\Delta n=\pm1$
	$F_c=0.32$		$F_c=\exp(-T/260)$	—	—
$CCl_3O_2NO_2+M \rightarrow CCl_3O_2+NO_2+M$	$1.5.10^{-17}$ [N_2] (k_0/s^{-1})	±0.3	$5.6\cdot10^{-4}\exp(-9310/T)$ [N_2]	260—300	±1000
	$1.6.10^{-1}$ (k_∞/s^{-1})	±0.3	$9.1.10^{14}\exp(-10820/T)\ s^{-1}$	260—300	±1000
	$F_c=0.20$				
$CH_2ClO_2NO_2+M \rightarrow CH_2ClO_2+NO_2+M$	см. [9]				

Table 2 (cont'd.)

Reaction	k_{298}, $cm^3\ s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3\ s^{-1}$	Temperatures range, K	$\Delta(E/R)$, K
		ClO_x reactions			
$O_3+C_2HCl_3\rightarrow$products	$<5\cdot10^{-20}$	—	—	—	—
$O_3+C_2Cl_4\rightarrow$products	$<10^{-21}$	—	—	—	—
$HOCl+h\nu\rightarrow$products	see Ref.9				
$OClO+h\nu\rightarrow$products	see Ref.9				
$Cl_2O_2+h\nu\rightarrow$products	see Ref.9				
$ClONO_2+h\nu\rightarrow$products	see Ref.9				
$COFCl+h\nu\rightarrow$products	see Ref.9				
$COCl_2+h\nu\rightarrow$products	see Ref.9				
$CF_2Cl_2+h\nu\rightarrow$products	see Ref.9				
$CFCl_3+h\nu\rightarrow$products	see Ref.9				
$CCl_4+h\nu\rightarrow$products					
		BrO_x reactions			
$O+HBr\rightarrow HO+Br$	$3.7\cdot10^{-14}$	±0.12	$6.6\cdot10^{-12}\exp(-1540/T)$	220—455	±200
$O+Br_2\rightarrow BrO+Br$	$1.4\cdot10^{-11}$	±0.2	—	—	—
$O+BrO\rightarrow O_2+Br$	$3\cdot10^{-11}$	±0.5	—	—	—
$Br+HO_2\rightarrow HBr+O_2$	$2.0\cdot10^{-12}$	±0.3	$1.4\cdot10^{-11}\exp(-590/T)$	260—390	±200
$Br+H_2O_2\rightarrow HBr+HO_2$ } $\rightarrow HOBr+HO$ }	$<5\cdot10^{-16}$	—	—	—	—
$Br+O_3\rightarrow BrO+O_2$	$1.2\cdot10^{-12}$	±0.1	$1.7\cdot10^{-11}\exp(-800/T)$	220—360	±200
$Br+HCHO\rightarrow HBr+HCO$	$1.0\cdot10^{-12}$	±0.15	$1.7\cdot10^{-11}\exp(-800/T)$	223—480	±250
$Br+CH_3CHO\rightarrow HBr+CH_3CO$	$3.6\cdot10^{-12}$	±0.2			
$Br+OClO\rightarrow BrO+ClO$	$3.4\cdot10^{-13}$	±0.3	$2.6\cdot10^{-11}\exp(-1300/T)$	200—450	±300
$HO+HBr\rightarrow H_2O+Br$	$1.1\cdot10^{-11}$	±0.1	$1.1\cdot10^{-11}$	249—416	±250
$HO+Br_2\rightarrow HOBr+Br$	$4.5\cdot10^{-11}$	±0.15	$1.2\cdot10^{-11}\exp(+400/T)$	260—360	±400
$HO+CH_3Br\rightarrow H_2O+CH_2Br$	$3.8\cdot10^{-14}$	±0.1	$7.6\cdot10^{-13}\exp(-890/T)$	244—350	±200
$BrO+HO_2\rightarrow HOBr+O_2$ } $\rightarrow HBr+O_3$ }	$5\cdot10^{-12}$	±0.5	—	—	—
$BrO+O_3\rightarrow Br+2O_2$	$<5\cdot10^{-15}$	—	—	—	—
$BrO+NO\rightarrow Br+NO_2$	$2.1\cdot10^{-11}$	±0.1	$8.7\cdot10^{-12}\exp(+260/T)$	224—425	±100
$BrO+NO_2+M\rightarrow BrONO_2+M$	$5.0\cdot10^{-31}[O_2]$ (k_0)	±0.3	$5.0\cdot10^{-31}(T/300)^{-3.0}[O_2]$	200—300	$\Delta n=\pm1$
	$5.0\cdot10^{-31}[N_2]$ (k_0)	±0.3	$5.0\cdot10^{-31}(T/300)^{-3.0}[N_2]$	200—300	$\Delta n=\pm1$
	$2\cdot10^{-11}$ (k_∞)	±0.3	$2\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.4$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/327)$	200—300	—
$BrO+ClO\rightarrow Br+OClO$	$6.9\cdot10^{-12}$	±0.1	$1.9\cdot10^{-12}\exp(+390/T)$	200—400	±400
$\rightarrow Br+ClOO$ } $\rightarrow BrCl+O_2$ }	$6.4\cdot10^{-12}$	±0.1	$3.9\cdot10^{-12}\exp(+140/T)$	200—400	±200
$BrO+BrO\rightarrow 2Br+O_2$	$2.2\cdot10^{-12}$	±0.1 }	$1.1\cdot10^{-12}\exp(+255/T)$	223—398	±300
$\rightarrow Br_2+O_2$	$4.5\cdot10^{-13}$	±0.2 }			
$HOBr+h\nu\rightarrow$products	см. [9]				
$BrO+h\nu\rightarrow$products	см. [9]				
$BrONO_2+h\nu\rightarrow$products	см. [9]				
		IO_x reactions			
$O+I_2\rightarrow IO+I$	$1.4\cdot10^{-10}$	±0.3	$1.4\cdot10^{-10}$	200—400	±250
$O+IO\rightarrow O_2+I$	$5\cdot10^{-11}$	±0.5	—	—	—
$I+HO_2\rightarrow HI+O_2$	no recommended value see Ref.9				
$I+O_3\rightarrow IO+O_2$	$9.5\cdot10^{-13}$	±0.2			
$I+NO+M\rightarrow INO+M$	$1.8\cdot10^{-32}[O_2]$ (k_0)	±0.2	$1.8\cdot10^{-32}(T/300)^{-1.0}[O_2]$	200—300	$\Delta n=\pm0.5$
	$1.8\cdot10^{-32}[N_2]$ (k_0)	±0.1	$1.8\cdot10^{-32}(T/300)^{-1.0}[N_2]$	200—300	$\Delta n=\pm0.5$
	$1.7\cdot10^{-11}$ (k_∞)	±0.3	$1.7\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.75$	$\Delta F_c=\pm0.15$	$F_c=\exp(-T/1043)$		
$I+NO_2+M\rightarrow INO_2+M$	$2.9\cdot10^{-31}[O_2]$ (k_0)	±0.3	$2.9\cdot10^{-31}(T/300)^{-1.0}[O_2]$	200—300	$\Delta n=\pm0.5$
	$2.9\cdot10^{-31}[N_2]$ (k_0)	±0.3	$2.9\cdot10^{-31}(T/300)^{-1.0}[N_2]$	200—300	$\Delta n=\pm0.5$
	$6.6\cdot10^{-11}$ (k_∞)	±0.3	$6.6\cdot10^{-11}$	200—300	$\Delta n=\pm0.5$
	$F_c=0.63$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/650)$	—	—
$HO+HI\rightarrow H_2O+I$	$1.3\cdot10^{-11}$	±0.5	—	—	—
$HO+I_2\rightarrow HOI+I$	$1.8\cdot10^{-10}$	±0.3	—	—	—
$IO+HO_2\rightarrow$products	no recommended value				
$IO+IO\rightarrow$products	$5.2\cdot10^{-11}$ (1 atm)	±0.5	$1.7\cdot10^{-12}\exp(+1020/T)$ (1 atm)	250—373	±200
$IO+NO\rightarrow I+NO_2$	$1.7\cdot10^{-11}$	±0.3	—	—	—
$IO+NO_2+M\rightarrow IONO_2+M$	$3.4\cdot10^{-31}[O_2]$ (k_0)	±0.5	$3.4\cdot10^{-31}(T/300)^{-3.0}[O_2]$	200—400	$\Delta n=\pm1$
	$3.4\cdot10^{-31}[N_2]$ (k_0)	±0.5	$3.4\cdot10^{-31}(T/300)^{3.0}[N_2]$	200—400	$\Delta n=\pm1$
	$1.6\cdot10^{-11}$ (k_∞)	±0.5	$1.6\cdot10^{-11}$	200—400	$\Delta n=\pm0.5$
	$F_c=0.4$	$\Delta F_c=\pm0.1$	$F_c=\exp(-T/327)$	—	—
$IO+CH_3SCH_3\rightarrow$products	no recommended value				
$INO+INO\rightarrow I_2+2NO$	$1.3\cdot10^{-14}$	±0.4	$8.4\cdot10^{-11}\exp(-2620/T)$	298—450	±600

Table 2 (cont'd.)

Reaction	k_{298}, $cm^3 s^{-1}$	$\Delta \lg k_{298}$	Temperature dependence of K, $cm^3 s^{-1}$	Temperatures range, K	$\Delta (E/R)$, K
			IO_x reactions		
$INO_2+NIO_2 \rightarrow I_2+2NO_2$	$4.7 \cdot 10^{-15}$	± 0.5	$2.9 \cdot 10^{-11} \exp(-2600/T)$	298—400	± 1000
$HOI+h\nu \rightarrow$ products	see Ref.9				
$IO+h\nu \rightarrow$ products	see Ref.9				
$INO+h\nu \rightarrow$ products	see Ref.9				
$INO_2+h\nu \rightarrow$ products	see Ref.9				
$IONO_2+h\nu \rightarrow$ products	see Ref.9				

3. Photochemical reactions

In CODATA/IUPAC reviews, tables of data begin with a list of the primary photochemical transitions at wavelengths not less than 170 nm. Also presented are the corresponding enthalpy changes at 0 K when this is possible, otherwise the values of 298 K are given. Also listed are the threshold wavelengths corresponding to these enthalpy changes. Next, the existing experimental data for the absorption cross-sections and quantum yields are compiled. These data are accompanied by commentaries. After that, the recommended absorption cross-sections and quantum yields for different wavelengths are listed wherever possible at 5 nm intervals. In many cases diagrams illustrating the dependence of the absorption cross-sections and quantum yields on the wavelength are shown as well. The choice of the recommended values is justified in the commentaries and certain other questions are considered.

4. Absorption cross-sections

In the CODATA/IUPAC compilations of data, these quantities are listed under the heading "absorption cross-sections per molecule to base e". They were determined in accordance with the equation

$$I/I_0 = \exp(-\sigma N l),$$
$$\sigma = (1/(Nl)) \cdot \ln(I_0/I),$$

where I_0 and I are the intensities of the incident and transmitted light, σ is the absorption cross-section (cm^2), N the number of particles of the absorbing substance (cm^{-3}) and l the distance traversed by the beam (cm). Other definitions and units of the measurement are also used. The closely related "absorption coefficient" and "extinction coefficients" are frequently quoted, but their definitions should not be confused. It is always necessary to draw attention to the units of the measurement of concentration, the traversed distance, and also the type of logarithm used in the definition (natural or decadic).

5. Determination of errors

The estimates of the absolute errors of the recommended values of k at 298 K and of the quantities E/R in the temperature range indicated are listed in the CODATA/IUPAC tables under the heading "reliability". These limits of errors are also given below in Table 2. The errors of the recommended rate constants at 298 K are expressed by the term

$$\Delta \lg k = D; \quad \lg k = C \pm D.$$

This is equivalent to the determination of k to within a multiplier F, where $D = \lg F$. The accuracy of the recommended values of E/R is expressed by the term $\Delta(E/R)$, where $\Delta(E/R) = G$ and G is defined by the equation $E/R = H \pm G$.

The absolute errors in k and E/R were determined by the Expert Panel. Experience has shown that, for the reactions of atoms and free radicals in the gas phase, the accuracy (reproducibility) of the measurements is usually good. Thus, for a separate investigation of a specified reaction by this method, the standard deviation (or even the 90% confidence interval) is, as stated in the literature, not more than $\pm 10\%$. Unfortunately, when data obtained by different groups of investigators using different methods for the same reaction are compared, it is frequently found that the rate constants differ by a factor of 2 or even more. This means that one or several investigations involve large systematic errors, which are difficult to detect. This is not surprising since, in contrast to molecular reactions, it is not always possible to investigate the reactions of atoms and radicals in isolation and hence experimental difficulties frequently arise.

The critical evaluations of errors in the CODATA/IUPAC selections are based mainly on the state of our knowledge for a particular reaction, which depends on the number of studies carried out and on the number of methods employed. Overall, the limits of error have been expanded. Thus in the case of a single study by one method not confirmed by independent investigations, limits of at least double errors indicated are adopted.

V. Table of reactions and recommended kinetic quantities

A complete list of chemical reactions and recommended kinetic parameters from the latest IUPAC survey is presented in Table 2. Unfortunately, it was not possible to present photochemical data in a compact form and we refer the reader to the complete CODATA/IUPAC publications[9].

* * *

At the time of the publication of the CODATA (Supplement 11)[39] and NASA (No. 7)[40] surveys, it was believed that the principal features of stratospheric gas-phase chemistry, including the constants of the key reactions, had been thoroughly established. At the present time additional requirements as regards the heterogeneous chemistry of polar stratospheric clouds, which may help to explain the appearance of Antarctic "ozone holes", must be added to this statement. A kinetic data bank for the chemistry of polar stratospheric clouds is being rapidly created at the present time, which should be reflected in extended surveys by both the NASA Group and the IUPAC Subcommittee for the Estimation of Gas-Kinetic Data for Atmospheric Chemistry. The second of these groups has begun to formulate a survey of kinetic data for reactions, mainly of organic species, which play a key role in the chemistry of the troposphere.

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