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REACTION RATE COEFFICIENTS FOR FLAME CALCULATIONS.(U)
JUL 77 D E JENSEN, G A JONES

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PROPELLANTS, EXPLOSIVES AND ROCKET MOTOR ESTABLISHMENT
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(6) REACTION RATE COEFFICIENTS FOR FLAME CALCULATIONS.

by

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SUMMARY

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A list of recommended rate coefficients for chemical reactions occurring in flames is given. Rate coefficients, expressed as functions of temperature for the range $1000 \leq T \leq 3000$ K, are either taken from experiments described in the scientific literature or estimated by comparison with rate coefficients for analogous reactions. Brief notes on the origins of recommended coefficients are included and rough uncertainties are attached to the listed values. A table showing reaction equilibrium constants as functions of temperature is also provided.

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CONTENTS

		Page
1	INTRODUCTION	5
2	LIST OF RATE COEFFICIENTS	9
3	NOTES ON RATE COEFFICIENTS	16
4	EQUILIBRIUM CONSTANTS AS FUNCTIONS OF TEMPERATURE	45
5	REFERENCES	51

1 INTRODUCTION

This report contains a list of chemical reaction rate coefficients compiled for use in calculations of flame structures. In many respects it is an up-dated version of a previous report[1], published in 1971, although the number of reactions considered is greatly increased. Many of the rate coefficient expressions recommended in 1971 are substantially revised in the light of work published during the past six years.

A major specific application of the data given in this report at PERME Westcott is to the calculation of electromagnetic properties (e.g. infrared and visible radiation characteristics, free electron content) of rocket exhaust flames, as illustrated in Ref. 2. Although this application was uppermost in the authors' minds when the list of recommendations was drawn up, the values given should nevertheless be found useful in a wide range of other combustion contexts, including those of MHD power generation, industrial burners, fire inhibition, combustion-driven lasers and turbine engines. The reactions for which rate coefficients are listed in this report in no sense constitute a reaction mechanism for any particular calculation: the reactions incorporated in the reaction scheme for such a calculation must always be selected in the light of the particular characteristics of the combustion system under consideration and the flame structure properties required.

Rate coefficients listed are defined in the manner usually adopted in descriptions of chemical rate processes. For example, the rate coefficient k of the reaction

$$aA + bB + cC \ldots \rightarrow a'A' + b'B' + c'C' \ldots$$

is defined by

$$k = -\frac{1}{a\,[A]^a\,[B]^b\,[C]^c \ldots}\,\frac{d\,[A]}{dt}$$

$$= -\frac{1}{b\,[A]^a\,[B]^b\,[C]^c \ldots}\,\frac{d\,[B]}{dt}$$

$$= \ldots\ldots\ldots$$

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The rate coefficient for the reverse reaction is similarly defined by

$$k' = -\frac{1}{a'[A']^{a'}[B']^{b'}[C']^{c'}\ldots}\frac{d[A']}{dt}$$

$$= -\frac{1}{b'[A']^{a'}[B']^{b'}[C']^{c'}\ldots}\frac{d[B']}{dt}$$

$$= \ldots\ldots\ldots$$

At equilibrium (when the reaction is balanced) the net rate of change of $[A]$, $[B]$, $[C]$ .... is zero. For species A , then

$$a\,k'[A']^{a'}[B']^{b'}[C']^{c'}\ldots - a\,k[A]^{a}[B]^{b}[C]^{c}\ldots = 0 \quad .$$

(Similar expressions arise from consideration of the net rates of change of $[B]$, $[C]$ ....) Hence

$$\frac{k}{k'} = \frac{[A']^{a'}[B']^{b'}[C']^{c'}\ldots}{[A]^{a}[B]^{b}[C]^{c}\ldots} = K \quad ,$$

where K is the equilibrium constant. Termolecular rate coefficients are expressed in units of ml^2 $molecule^{-2}$ s^{-1} and bimolecular rate coefficients in ml $molecule^{-1}$ s^{-1}. All temperatures are expressed in Kelvins.

The rate coefficients given are based, wherever possible, on experimental measurements. Where no measurements are available (as applies to a large number of reactions), coefficients are estimated by comparison with those for similar reactions, allowances being made in the light of collision and transition state theories for probable steric, reduced mass and cross section differences. Although recent progress on theoretical calculations of unmeasured rate coefficients has been encouraging, such handicaps as the lack of accurate molecular configurations and potential energy surfaces for transition states make it difficult to justify a more rigorous approach at present. It is urged that under no circumstances should the reader make use of a rate coefficient given in this report without considering the comment indicating the source of the value.

The rate coefficients are intended for use in calculations on combustion systems at temperatures between 1000 and 3000 K. Extrapolations outside this temperature regime, especially to lower temperatures, should be made only with extreme caution. The "Arrhenius" forms in which k and K are expressed merely provide convenient empirical fits for the specified temperature range. In nearly all cases, however, the experimental data are not accurate enough to warrant a more complicated form of expression for this range.

The uncertainty factor UF given for each rate coefficient is such that $k \times UF$ and k/UF provide probable approximate upper and lower bounds respectively to k at that temperature within the range 1000-3000 Kelvins for which the rate coefficient is least accurately known. These uncertainty factors, intended to give the user a feeling for the precision of the listed rate coefficients, are the result of broad semi-quantitative appraisal rather than detailed statistical analysis of the available data, and are consequently rather subjective. Uncertainty factors of 10 or 100 appear frequently, as do those of 30; this last value is intended to convey nothing more precise than that UF is greater than 10 but less than 100. Large uncertainty bounds associated with the rate coefficient of a given reaction do not necessarily imply that there may be substantial errors in calculations involving this reaction. On the one hand, a reaction with large uncertainty limits in its rate coefficient may in any case be so fast that it is very close to chemical equilibrium; on the other, a different reaction, also with large rate uncertainties, may in any case be so slow that it is overwhelmed by concomitant mixing processes. The uncertainty factors are often much larger than those attached to their results by the original experimenters, usually because it has been necessary in this report to extrapolate available results into temperature ranges widely different from those of the experiments themselves.

Two particularly difficult points in the description of chemical kinetics arise in the case of the reactions involving "third bodies" or "collision partners" M (e.g. those in groups A and G). The first is that different third bodies have different (and sometimes unknown) efficiencies in these reactions. Here an attempt is made to give rate coefficients averaged for the more effective third bodies (e.g. CO_2 , H_2O , N_2) in a typical flame. The concentration $[M]$ is then taken as the sum of concentrations of all gas phase species present. The deficiencies of this approach are clear; our defence of its use is that the errors which it introduces are usually (although not always) small by comparison with possible errors in the rate coefficients for individual third bodies. A

second difficulty is that the third body reactions (and their reverse reactions) actually take place via stepwise processes involving excited molecular or atomic states, vibrational and electronic. Consequently the reverse reactions often have overall rate coefficients much higher than the "collision frequency". One should really take account of individual reactions of these states rather than choose, as here, overall rate coefficients for overall - and, in a sense, artificial - reactions. Fundamental data currently available are insufficient for dealing with this problem. Alternative formal descriptions of the chemical rate processes occurring in flames (e.g. those in terms of cross sections expressed as functions of molecular energy rather than in terms of rate coefficients expressed as functions of temperature), which in the future may resolve this difficulty, lead at present to even greater problems.

The "collision frequencies" to which kineticists often refer rate coefficients are generally those calculated on the assumption that all chemical species are in ground electronic, vibrational and rotational states, although this common usage is sometimes rather misleading. The simplest collision theory expression for a bimolecular rate coefficient k is

$$k = p \pi \sigma^2 (8 \kappa T/\pi \mu)^{\frac{1}{2}} \exp(-E/\kappa T)$$

where p is a "steric" or "probability" factor, $\pi \sigma^2$ the collision cross section, κ the Boltzmann constant, μ the reduced mass and E the activation energy. The product $p \pi \sigma^2 (8 \kappa T/\pi \mu)^{\frac{1}{2}}$ is termed the pre-exponential factor, and $\pi \sigma^2 (8 \kappa T/\pi \mu)^{\frac{1}{2}}$ is (loosely) called the collision frequency, even though p and $\pi \sigma^2$ are experimentally inseparable. For a typical reaction with reduced mass 2.5×10^{-23} g and collision cross section 3×10^{-19} m^2 at 1600 K, the collision frequency is 5×10^{-10} ml molecule^{-1} sec^{-1}. Thus a pre-exponential factor of 5×10^{-10} ml molecule^{-1} sec^{-1} would, on this terminology, imply a steric factor of unity.

The values of rate coefficients given are considered to be the best that can be gleaned from the literature published up to the end of 1976, although a few later references are given. The notes on sources of data are brief and the list of references far from complete: much valuable kinetic work is not acknowledged or discussed in order that the report should remain relatively short.

The rate quotient law (which states that the ratio of the rate coefficient k_i of the forward reaction to the rate coefficient k_{-i} of the backward reaction is equal to the equilibrium constant K_i, and apparent deviations from which arise only from inadequate descriptions of rate processes) is assumed to hold for all reactions. Occasional difficulties, the source of which is noted above, result from this assumption for the overall reactions of type $A + B + M \rightleftharpoons AB + M$, but these difficulties must be accepted at present. The equilibrium constants listed are deliberately set in a form that makes it easy to determine the implied pre-exponential factor and activation energy in k_{-i} from the tabulated value of k_i. This form introduces some small errors in K_i at the extremes of the temperature range considered (up to almost a factor of 2 in some cases), but the uncertainty factors in both k_i and k_{-i} are almost always much larger than the errors so incurred.

The method of numbering reactions is retained from Ref. 1. It keeps arbitrarily related reactions in groups and enables one to add reactions conveniently as new data become available.

2 LIST OF RATE COEFFICIENTS

Bimolecular rate coefficients are in units of ml molecule^{-1} sec^{-1}; termolecular rate coefficients in ml^2 molecule^{-2} sec^{-1}.

Reaction	Number	Rate Coefficient	Uncertainty Factor
$O + O + M \rightarrow O_2 + M$	A1	$3 \times 10^{-34} \exp(+900/T)$	10
$O + H + M \rightarrow OH + M$	A2	$1 \times 10^{-29} T^{-1}$	30
$H + H + M \rightarrow H_2 + M$	A3	$3 \times 10^{-30} T^{-1}$	30
$H + OH + M \rightarrow H_2O + M$	A4	$2 \times 10^{-25} T^{-2}$	10
$CO + O + M \rightarrow CO_2 + M$	A5	$7 \times 10^{-33} \exp(-2200/T)$	30
$OH + H_2 \rightarrow H_2O + H$	B1	$3.6 \times 10^{-11} \exp(-2600/T)$	2
$O + H_2 \rightarrow OH + H$	B2	$3.0 \times 10^{-14} T \exp(-4480/T)$	1.5
$H + O_2 \rightarrow OH + O$	B3	$3.7 \times 10^{-10} \exp(-8450/T)$	1.5
$CO + OH \rightarrow CO_2 + H$	B4	$2.8 \times 10^{-17} T^{1.3} \exp(330/T)$	3
$OH + OH \rightarrow H_2O + O$	B5	$1 \times 10^{-11} \exp(-550/T)$	3
$CO + O_2 \rightarrow CO_2 + O$	B6	$4.2 \times 10^{-12} \exp(-24000/T)$	3
$H + Cl_2 \rightarrow HCl + Cl$	C1	$1.4 \times 10^{-10} \exp(-250/T)$	10
$Cl + H_2 \rightarrow HCl + H$	C2	$1.4 \times 10^{-11} \exp(-2130/T)$	5
$H_2O + Cl \rightarrow HCl + OH$	C3	$1.6 \times 10^{-10} \exp(-9100/T)$	10
$OH + Cl \rightarrow HCl + O$	C4	$4 \times 10^{-12} \exp(-2500/T)$	30
$H + HF \rightarrow H_2 + F$	C5	$7 \times 10^{-11} \exp(-16500/T)$	30
$H + F_2 \rightarrow HF + F$	C6	$1 \times 10^{-10} \exp(-700/T)$	10
$Li + HCl \rightarrow LiCl + H$	D1	$2 \times 10^{-10} \exp(-500/T)$	30
$Na + HCl \rightarrow NaCl + H$	D2	$2 \times 10^{-10} \exp(-4000/T)$	30
$K + HCl \rightarrow KCl + H$	D3	$3 \times 10^{-10} \exp(-2500/T)$	30
$Li + H_2O \rightarrow LiOH + H$	D4	$6 \times 10^{-11} \exp(-11000/T)$	30
$Na + H_2O \rightarrow NaOH + H$	D5	$8 \times 10^{-11} \exp(-22000/T)$	30
$K + H_2O \rightarrow KOH + H$	D6	$1 \times 10^{-10} \exp(-20000/T)$	30
$K + HBO_2 \rightarrow KBO_2 + H$	D7	$2 \times 10^{-10} \exp(-4200/T)$	30
$K + H_2WO_4 \rightarrow KHWO_4 + H$	D8	$2 \times 10^{-10} \exp(-500/T)$	30
$K + H_2MoO_4 \rightarrow KHMoO_4 + H$	D9	$2 \times 10^{-10} \exp(-500/T)$	30
$Na + HBO_2 \rightarrow NaBO_2 + H$	D10	$1 \times 10^{-10} \exp(-5000/T)$	30
$Li + HBO_2 \rightarrow LiBO_2 + H$	D11	$1 \times 10^{-10} \exp(-1000/T)$	30
$Cs + H_2O \rightarrow CsOH + H$	D12	$2 \times 10^{-10} \exp(-18000/T)$	30
$H + Cl + M \rightarrow HCl + M$	E1	$4 \times 10^{-26} T^{-2}$	100
$Cl + Cl + M \rightarrow Cl_2 + M$	E2	$2 \times 10^{-33} \exp(900/T)$	30
$H + F + M \rightarrow HF + M$	E3	$3 \times 10^{-29} T^{-1}$	30
$F + F + M \rightarrow F_2 + M$	E4	$3 \times 10^{-30} T^{-1.5}$	100
$Li + OH + M \rightarrow LiOH + M$	F1	$3 \times 10^{-28} T^{-1}$	30
$Na + OH + M \rightarrow NaOH + M$	F2	$5 \times 10^{-28} T^{-1}$	30
$K + OH + M \rightarrow KOH + M$	F3	$6 \times 10^{-28} T^{-1}$	30
$Li + Cl + M \rightarrow LiCl + M$	F4	$2 \times 10^{-28} T^{-1}$	30
$Na + Cl + M \rightarrow NaCl + M$	F5	$3 \times 10^{-28} T^{-1}$	30
$K + Cl + M \rightarrow KCl + M$	F6	$5 \times 10^{-28} T^{-1}$	30

Reaction	Number	Rate Coefficient	Uncertainty Factor
$Li^+ + e^- + M \rightarrow Li + M$	G1	$4 \times 10^{-24}\ T^{-1}$	5
$Na^+ + e^- + M \rightarrow Na + M$	G2	$4 \times 10^{-24}\ T^{-1}$	5
$K^+ + e^- + M \rightarrow K + M$	G3	$4 \times 10^{-24}\ T^{-1}$	5
$Cs^+ + e^- + M \rightarrow Cs + M$	G4	$4 \times 10^{-24}\ T^{-1}$	5
$In^+ + e^- + M \rightarrow In + M$	G5	$6 \times 10^{-21}\ T^{-2}$	10
$Li^+ + Cl^- \rightarrow Li + Cl$	H1	$7.6 \times 10^{-8}\ T^{-0.5}$	10
$Na^+ + Cl^- \rightarrow Na + Cl$	H2	$2.2 \times 10^{-8}\ T^{-0.5}$	10
$K^+ + Cl^- \rightarrow K + Cl$	H3	$1.7 \times 10^{-9}\ T^{-0.5}$	10
$Li^+ + OH^- \rightarrow Li + OH$	H4	$1 \times 10^{-8}\ T^{-0.5}$	100
$Na^+ + OH^- \rightarrow Na + OH$	H5	$1 \times 10^{-8}\ T^{-0.5}$	100
$K^+ + OH^- \rightarrow K + OH$	H6	$1 \times 10^{-8}\ T^{-0.5}$	100
$Li^+ + Cl^- + M \rightarrow LiCl + M$	H7	$1.2 \times 10^{-15}\ T^{-3.5}\ \exp(-300/T)$	10
$Na^+ + Cl^- + M \rightarrow NaCl + M$	H8	$5.5 \times 10^{-16}\ T^{-3.5}\ \exp(-750/T)$	10
$K^+ + Cl^- + M \rightarrow KCl + M$	H9	$1.6 \times 10^{-15}\ T^{-3.5}\ \exp(-2400/T)$	10
$OH + e^- + M \rightarrow OH^- + M$	J1	3×10^{-31}	100
$Cl + e^- + M \rightarrow Cl^- + M$	J2	$1 \times 10^{-32}\ \exp(3000/T)$	30
$HCl + e^- \rightarrow Cl^- + H$	J3	$1.4 \times 10^{-7}\ \exp(-7600/T)$	10
$HBO_2 + e^- \rightarrow BO_2^- + H$	J4	$1 \times 10^{-8}\ \exp(-11000/T)$	100
$H_2MoO_4 + e^- \rightarrow HMoO_4^- + H$	J5	$1 \times 10^{-8}\ \exp(-1500/T)$	100
$H_2WO_4 + e^- \rightarrow HWO_4^- + H$	J6	$1 \times 10^{-8}\ \exp(-1000/T)$	100
$H_2O + e^- \rightarrow OH^- + H$	J7	$1 \times 10^{-8}\ \exp(-35000/T)$	100
$HMoO_4^- + H \rightarrow MoO_3^- + H_2O$	J8	1×10^{-9}	30
$HWO_4^- + H \rightarrow WO_3^- + H_2O$	J9	1×10^{-9}	30
$O_2 + e^- + M \rightarrow O_2^- + M$	J10	1×10^{-30}	30
$LiH_2O^+ + M \rightarrow Li^+ + H_2O + M$	L1	$2 \times 10^{-7}\ \exp(-23000/T)$	100
$NaH_2O^+ + M \rightarrow Na^+ + H_2O + M$	L2	$3 \times 10^{-7}\ \exp(-15000/T)$	100
$KH_2O^+ + M \rightarrow K^+ + H_2O + M$	L3	$1 \times 10^{-7}\ \exp(-10000/T)$	100
$LiH_2O^+ + e^- \rightarrow Li + H_2O$	L4	1×10^{-7}	30
$NaH_2O^+ + e^- \rightarrow Na + H_2O$	L5	1×10^{-7}	30
$KH_2O^+ + e^- \rightarrow K + H_2O$	L6	1×10^{-7}	30
$LiH_2O^+ + Cl^- \rightarrow Li + Cl + H_2O$	L7	4×10^{-8}	100
$NaH_2O^+ + Cl^- \rightarrow Na + Cl + H_2O$	L8	4×10^{-8}	100
$KH_2O^+ + Cl^- \rightarrow K + Cl + H_2O$	L9	4×10^{-8}	100
$LiH_2O^+ + OH^- \rightarrow Li + OH + H_2O$	L10	4×10^{-8}	100
$NaH_2O^+ + OH^- \rightarrow Na + OH + H_2O$	L11	4×10^{-8}	100
$KH_2O^+ + OH^- \rightarrow K + OH + H_2O$	L12	4×10^{-8}	100

Reaction	Number	Rate Coefficient	Uncertainty Factor
$Cl + O + M \rightarrow ClO + M$	M1	$1 \times 10^{-29}\ T^{-1}$	100
$Li + ClO \rightarrow LiCl + O$	M2	$2 \times 10^{-10}\ \exp(-1500/T)$	100
$Na + ClO \rightarrow NaCl + O$	M3	$3 \times 10^{-10}\ \exp(-1500/T)$	100
$K + ClO \rightarrow KCl + O$	M4	$3 \times 10^{-10}\ \exp(-1500/T)$	100
$ClO + H \rightarrow HCl + O$	M5	$1 \times 10^{-10}\ \exp(-500/T)$	30
$ClO + O \rightarrow Cl + O_2$	M6	$1.1 \times 10^{-10}\ \exp(-220/T)$	5
$ClO + OH \rightarrow Cl + HO_2$	M7	$1.3 \times 10^{-11}\ \exp(-1380/T)$	30
$Li + O_2 + M \rightarrow LiO_2 + M$	N1	$1 \times 10^{-30}\ T^{-1}$	100
$Na + O_2 + M \rightarrow NaO_2 + M$	N2	$1 \times 10^{-30}\ T^{-1}$	10
$K + O_2 + M \rightarrow KO_2 + M$	N3	$1 \times 10^{-30}\ T^{-1}$	10
$LiO_2 + Cl \rightarrow LiCl + O_2$	N4	$1 \times 10^{-10}\ \exp(-1000/T)$	30
$NaO_2 + Cl \rightarrow NaCl + O_2$	N5	$1 \times 10^{-10}\ \exp(-1000/T)$	30
$KO_2 + Cl \rightarrow KCl + O_2$	N6	$1 \times 10^{-10}\ \exp(-1000/T)$	30
$LiO_2 + H_2 \rightarrow LiOH + OH$	N7	$3 \times 10^{-12}\ \exp(-10000/T)$	100
$NaO_2 + H_2 \rightarrow NaOH + OH$	N8	$3 \times 10^{-12}\ \exp(-10000/T)$	100
$KO_2 + H_2 \rightarrow KOH + OH$	N9	$3 \times 10^{-12}\ \exp(-10000/T)$	100
$LiO_2 + OH \rightarrow LiOH + O_2$	N10	2×10^{-11}	30
$NaO_2 + OH \rightarrow NaOH + O_2$	N11	2×10^{-11}	30
$KO_2 + OH \rightarrow KOH + O_2$	N12	2×10^{-11}	30
$Na(^2S_{1/2}) + H + OH \rightarrow Na(^2P_{1/2}) + H_2O$	N13	1×10^{-31}	30
$Na(^2S_{1/2}) + H + OH \rightarrow Na(^2P_{3/2}) + H_2O$	N14	1×10^{-31}	30
$Na(^2S_{1/2}) + H + H \rightarrow Na(^2P_{1/2}) + H_2$	N15	1×10^{-31}	30
$Na(^2S_{1/2}) + H + H \rightarrow Na(^2P_{3/2}) + H_2$	N16	1×10^{-31}	30
$Na(^2S_{1/2}) + O + O \rightarrow Na(^2P_{1/2}) + O_2$	N17	5×10^{-30}	100
$Na(^2S_{1/2}) + O + O \rightarrow Na(^2P_{3/2}) + O_2$	N18	5×10^{-30}	100
$Na(^2S_{1/2}) + M \rightarrow Na(^2P_{1/2}) + M$	N19	$1.2 \times 10^{-11}\ T^{0.5}\ \exp(-24400/T)$	5
$Na(^2S_{1/2}) + M \rightarrow Na(^2P_{3/2}) + M$	N20	$2.4 \times 10^{-11}\ T^{0.5}\ \exp(-24400/T)$	5
$Na(^2P_{1/2}) + M \rightarrow Na(^2P_{3/2}) + M$	N24	3×10^{-10}	5
$K(^2S_{1/2}) + H + OH \rightarrow K(^2P_{1/2}) + H_2O$	N25	1×10^{-31}	100
$K(^2S_{1/2}) + H + OH \rightarrow K(^2P_{3/2}) + H_2O$	N26	1×10^{-31}	100
$K(^2S_{1/2}) + H + H \rightarrow K(^2P_{1/2}) + H_2$	N27	1×10^{-31}	100
$K(^2S_{1/2}) + H + H \rightarrow K(^2P_{3/2}) + H_2$	N28	1×10^{-31}	100
$K(^2S_{1/2}) + O + O \rightarrow K(^2P_{1/2}) + O_2$	N29	5×10^{-30}	100
$K(^2S_{1/2}) + O + O \rightarrow K(^2P_{3/2}) + O_2$	N30	5×10^{-30}	100
$K(^2S_{1/2}) + M \rightarrow K(^2P_{1/2}) + M$	N31	$1.2 \times 10^{-11}\ T^{0.5}\ \exp(-18690/T)$	5
$K(^2S_{1/2}) + M \rightarrow K(^2P_{3/2}) + M$	N32	$2.4 \times 10^{-11}\ T^{0.5}\ \exp(-18820/T)$	5
$K(^2P_{1/2}) + M \rightarrow K(^2P_{3/2}) + M$	N35	$3 \times 10^{-10}\ \exp(-200/T)$	10
$Na + HO_2 \rightarrow NaO_2 + H$	N38	$1 \times 10^{-11}\ \exp(-1000/T)$	30
$K + HO_2 \rightarrow KO_2 + H$	N41	$1 \times 10^{-11}\ \exp(-1000/T)$	30

Reaction	Number	Rate Coefficient	Uncertainty Factor
$H + O_2 + M \rightarrow HO_2 + M$	P1	$2 \times 10^{-32} \exp(500/T)$	10
$Cl + HO_2 \rightarrow HCl + O_2$	P2	$1.2 \times 10^{-10} \exp(-480/T)$	10
$H + HO_2 \rightarrow OH + OH$	P3	$4 \times 10^{-10} \exp(-950/T)$	5
$H + HO_2 \rightarrow H_2 + O_2$	P4	$4 \times 10^{-11} \exp(-350/T)$	5
$H_2 + HO_2 \rightarrow H_2O + OH$	P5	$1 \times 10^{-12} \exp(-9400/T)$	10
$CO + HO_2 \rightarrow CO_2 + OH$	P6	$2.5 \times 10^{-10} \exp(-11900/T)$	10
$O + HO_2 \rightarrow OH + O_2$	P7	$8 \times 10^{-11} \exp(-500/T)$	30
$OH + HO_2 \rightarrow H_2O + O_2$	P8	1×10^{-10}	30
$CHO + O \rightarrow CO + OH$	Q1	$3 \times 10^{-11} \exp(-2500/T)$	100
$CHO + OH \rightarrow CO + H_2O$	Q2	1×10^{-11}	100
$CO + H + M \rightarrow CHO + M$	Q3	$2 \times 10^{-33} \exp(-850/T)$	100
$CHO + H \rightarrow CO + H_2$	Q4	$2 \times 10^{-10} \exp(-2500/T)$	30
$CH_4 + H \rightarrow CH_3 + H_2$	Q5	$7 \times 10^{-10} \exp(-7500/T)$	30
$CH_4 + O \rightarrow CH_3 + OH$	Q6	$5 \times 10^{-11} \exp(-4500/T)$	5
$CH_4 + OH \rightarrow CH_3 + H_2O$	Q7	$5 \times 10^{-11} \exp(-2500/T)$	5
$CH_2O + OH \rightarrow CHO + H_2O$	Q8	$1 \times 10^{-10} \exp(-500/T)$	100
$CH_2O + H \rightarrow CHO + H_2$	Q9	$5 \times 10^{-11} \exp(-2100/T)$	30
$CH_2O + O \rightarrow CHO + OH$	Q10	$2 \times 10^{-10} \exp(-2200/T)$	30
$CH_3 + OH \rightarrow CH_2O + H_2$	Q11	7×10^{-12}	100
$CH_3 + O_2 \rightarrow CH_2O + OH$	Q12	$5 \times 10^{-13} \exp(-5500/T)$	100
$CH_3 + O \rightarrow CH_2O + H$	Q13	$1 \times 10^{-10} \exp(-500/T)$	100
$CH_3 + H + M \rightarrow CH_4 + M$	Q14	$2 \times 10^{-21} T^{-3}$	100
$CH_3 + CH_3 \rightarrow C_2H_6$	Q15	$1 \times 10^{-11} \exp(500/T)$	30
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	Q16	$5 \times 10^{-17} T^2 \exp(-3500/T)$	10
$C_2H_5 + H \rightarrow C_2H_4 + H_2$	Q17	8×10^{-11}	100
$C_2H_4 + H \rightarrow C_2H_3 + H_2$	Q18	$3 \times 10^{-11} \exp(-3500/T)$	10
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	Q19	7×10^{-12}	30
$C_2H_2 + H \rightarrow C_2H + H_2$	Q20	$3 \times 10^{-10} \exp(-9500/T)$	1000
$C_2H + H \rightarrow C_2 + H_2$	Q21	$4 \times 10^{-11} \exp(-18000/T)$	100
$C_2H_4 + H \rightarrow C_2H_5$	Q22	$4 \times 10^{-12} \exp(-500/T)$	30
$C_2H_2 + H + M \rightarrow C_2H_3 + M$	Q23	$1 \times 10^{-33} \exp(4800/T)$	100
$C_2 + H + M \rightarrow C_2H + M$	Q24	$1 \times 10^{-28} T^{-1}$	100
$CHO + O_2 \rightarrow CO + HO_2$	Q25	$2 \times 10^{-10} \exp(-2000/T)$	30
$CH_3 + O \rightarrow CH + H_2O$	Q26	$5 \times 10^{-11} \exp(-1000/T)$	100
$Cl + OH + M \rightarrow HOCl + M$	R1	$1 \times 10^{-29} T^{-1}$	100
$HOCl + H \rightarrow ClO + H_2$	R2	1×10^{-11}	100
$HOCl + OH \rightarrow ClO + H_2O$	R3	3×10^{-12}	100
$HOCl + O \rightarrow ClO + OH$	R4	2×10^{-11}	100

Reaction	Number	Rate Coefficient	Uncertainty Factor
$CaOH^+ + e^- \rightarrow Ca + OH$	S1	$0.5\ T^{-2}$	5
$CaOH + H \rightarrow CaO + H_2$	S2	$4 \times 10^{-11}\ exp(-3680/T)$	30
$CaOH + H \rightarrow Ca + H_2O$	S3	$4 \times 10^{-12}\ exp(-600/T)$	30
$Ca + HCl \rightarrow CaCl + H$	S4	$3 \times 10^{-10}\ exp(-5000/T)$	30
$CaCl_2 + H \rightarrow CaCl + HCl$	S5	$1 \times 10^{-10}\ exp(-5000/T)$	30
$Ca(OH)_2 + H \rightarrow CaOH + H_2O$	S6	$3 \times 10^{-11}\ exp(-600/T)$	30
$CaO + H_2O \rightarrow Ca(OH)_2$	S7	6×10^{-10}	30
$CaOH^+ + e^- \rightarrow CaO + H$	S8	$0.5\ T^{-2}$	5
$CaOH^+ + H \rightarrow Ca^+ + H_2O$	S9	$1 \times 10^{-10}\ exp(-1000/T)$	30
$BaOH + H \rightarrow Ba + H_2O$	S21	$4 \times 10^{-12}\ exp(-500/T)$	30
$BaO + H_2O \rightarrow Ba(OH)_2$	S22	3×10^{-12}	30
$BaOH + H \rightarrow BaO + H_2$	S23	$3 \times 10^{-11}\ exp(-800/T)$	10
$Ba(OH)_2 + H \rightarrow BaOH + H_2O$	S24	$1 \times 10^{-10}\ exp(-300/T)$	30
$BaOH^+ + e^- \rightarrow Ba + OH$	S25	1×10^{-7}	10
$BaOH^+ + e^- \rightarrow BaO + H$	S26	1×10^{-7}	10
$BaOH^+ + H \rightarrow Ba^+ + H_2O$	S27	$1 \times 10^{-10}\ exp(-1000/T)$	30
$CH + O \rightarrow CHO^+ + e^-$	T3	$5 \times 10^{-9}\ T^{-1}\ exp(-1700/T)$	100
$CHO^+ + H_2O \rightarrow H_3O^+ + CO$	T4	1×10^{-8}	10
$H_3O^+ + Li \rightarrow Li^+ + H_2O + H$	T5	$1.7 \times 10^{-5}\ T^{-1}$	5
$H_3O^+ + Na \rightarrow Na^+ + H_2O + H$	T6	$4 \times 10^{-2}\ T^{-2}$	5
$H_3O^+ + K \rightarrow K^+ + H_2O + H$	T7	$4.5 \times 10^{-2}\ T^{-2}$	5
$H_3O^+ + In \rightarrow In^+ + H_2O + H$	T8	1×10^{-8}	10
$H_3O^+ + Cl^- \rightarrow H_2O + H + Cl$	T9	$7 \times 10^{-5}\ T^{-1}$	10
$H_3O^+ + OH^- \rightarrow H + OH + H_2O$	T10	8×10^{-8}	30
$H_3O^+ + e^- \rightarrow H + H + OH$	T11	$6 \times 10^{-4}\ T^{-1}$	5
$NO + NO \rightarrow N_2O + O$	U1	$2.2 \times 10^{-12}\ exp(-32100/T)$	5
$N_2O + H \rightarrow N_2 + OH$	U2	$1.3 \times 10^{-10}\ exp(-7600/T)$	3
$NO + H + M \rightarrow HNO + M$	U3	$1.5 \times 10^{-32}\ exp(300/T)$	10
$HNO + H \rightarrow NO + H_2$	U4	8×10^{-12}	10
$HNO + OH \rightarrow NO + H_2O$	U5	6×10^{-11}	5
$N_2 + O \rightarrow NO + N$	U6	$1.3 \times 10^{-10}\ exp(-38000/T)$	5
$N + O_2 \rightarrow NO + O$	U7	$1.1 \times 10^{-14}\ T\ exp(-3150/T)$	3

Reaction	Number	Rate Coefficient	Uncertainty Factor
$Fe + H_2O \rightarrow FeOH + H$	V1	$1.3 \times 10^{-10}\ \exp(-16700/T)$	30
$FeOH + H \rightarrow FeO + H_2$	V2	$5 \times 10^{-11}\ \exp(-800/T)$	30
$FeO + H_2O \rightarrow Fe(OH)_2$	V3	9×10^{-12}	10
$Fe(OH)_2 + H \rightarrow FeOH + H_2O$	V4	$1.1 \times 10^{-10}\ \exp(-300/T)$	10
$HMoO_3 + H \rightarrow MoO_3 + H_2$	V11	$1.1 \times 10^{-10}\ \exp(-1400/T)$	10
$MoO_3 + H_2O \rightarrow H_2MoO_4$	V12	1×10^{-11}	30
$H_2MoO_4 + H \rightarrow HMoO_3 + H_2O$	V13	$1.4 \times 10^{-10}\ \exp(-300/T)$	30
$HWO_3 + H \rightarrow WO_3 + H_2$	V21	$1.1 \times 10^{-10}\ \exp(-1000/T)$	10
$WO_3 + H_2O \rightarrow H_2WO_4$	V22	1×10^{-10}	30
$H_2WO_4 + H \rightarrow HWO_3 + H_2O$	V23	$3 \times 10^{-10}\ \exp(-1000/T)$	30
$Co + OH \rightarrow CoO + H$	V31	$1 \times 10^{-10}\ \exp(-1000/T)$	30
$CoOH + H \rightarrow CoO + H_2$	V32	$2 \times 10^{-10}\ \exp(-800/T)$	100
$CoO + H_2O \rightarrow Co(OH)_2$	V33	3×10^{-13}	30
$Co(OH)_2 + H \rightarrow CoOH + H_2O$	V34	$4 \times 10^{-10}\ \exp(-300/T)$	100
$H + H(+ Cr) \rightarrow H_2(+ Cr)$	V41	2×10^{-27}	100
$H + H(+ SnO) \rightarrow H_2(+ SnO)$	V42	5×10^{-28}	100

3 NOTES ON RATE COEFFICIENTS

A1 Baulch, Drysdale, Duxbury and Grant[3] recommend $k_{A1} = 5.2 \times 10^{-35} \exp(900/T)$ ml^2 $molecule^{-2}$ s^{-1} and $k_{-A1} = 3.0 \times 10^{-6} T^{-1} \exp(-59380/T)$ ml $molecule^{-1}$ s^{-1}, both for $M \equiv Ar$. In combination with our value for the equilibrium constant K_{A1}, the latter expression yields $k_{A1} = 2 \times 10^{-31} T^{-1} \exp(200/T)$ ml^2 $molecule^{-2}$ s^{-1}, agreeing with the recommendation $5 \times 10^{-35} \exp(900/T)$ ml^2 $molecule^{-2}$ s^{-1} to better than a factor of 2 throughout the temperature range of interest. For $M \equiv$ such other flame molecules as N_2, CO_2 and H_2, values of k_{A1} are typically some 3 to 10 times higher[3]. The listed value of k_{A1} appears to be a reasonable selection for use in flame calculations.

A2 Baulch, Drysdale, Horne and Lloyd[4] decline to make a recommendation for k_{A2} because of the lack of experimental data. The estimate of Ref. 1 is retained here.

A3 A great deal of experimental work has been done on this reaction, but the results are scattered and appear to show substantial variations from one third body to another[4]. Baulch, Drysdale, Horne and Lloyd[4] suggest $k_{A3} = 8.3 \times 10^{-33}$ ml^2 $molecule^{-2}$ s^{-1} at 300 K for $M \equiv H_2$ and $k_{-A3} = 3.7 \times 10^{-10} \exp(-48300/T)$ ml $molecule^{-1}$ s^{-1} for $M \equiv Ar$. The listed value is a compromise for use in flame calculations. Work published since 1972 does not suggest a value for k_{A3} significantly different from that listed for the "typical" flame third body.

A4 Baulch, Drysdale, Horne and Lloyd[4] recommend $k_{A4} = 3.9 \times 10^{-25} T^{-2}$ ml^2 $molecule^{-2}$ s^{-1} for $M \equiv H_2O$, and suggest that other third bodies are somewhat less effective in inducing recombination than is H_2O. A value of $2 \times 10^{-25} T^{-2}$ ml^2 $molecule^{-2}$ s^{-1} is adopted for flame calculations; this is in reasonable agreement with measurements on the reverse reaction[4]. Work published since 1972 does not suggest a value of k_{A4} significantly different from that listed for a "typical" flame third body.

A5 Baulch, Drysdale, Duxbury and Grant[3] suggest $k_{A5} = 6.5 \times 10^{-33} \exp(-2184/T)$ ml^2 $molecule^{-2}$ s^{-1} for $M \equiv CO$. In the light of the scattered results for other third bodies[3], this is a reasonable value to adopt for flame calculations.

B1 The listed value is taken from Ref. 4.

B2 The listed value is taken from Ref. 4.

B3 The listed value is taken from Ref. 4.

B4 This rate coefficient is selected to fit data collected in Ref. 3.

B5 The listed value is taken from Ref. 4.

B6 The listed value is taken from Ref. 3.

C1 The values of k_{C1} to be found in the literature (e.g. Refs 6-12) vary widely. That listed weights heavily the recent results of Bemand and Clyne[10] and Wagner, Welzbacher and Zellner[12], which agree well with one another.

C2 Ambidge, Bradley and Whytock[13] give $k_{-C2} = 8 \times 10^{-12} \exp(-1600/T)$ ml molecule^{-1} s^{-1}. These authors also account for a previous apparent discrepancy[14] between measurements of the rate coefficients for the forward and backward steps of this reaction. The value of Ref. 13 is adopted. It is in reasonable agreement with previous work.

C3 Takacs and Glass[15], Anderson, Zahniser and Kaufman[16] and Smith and Zellner[17] all find k_{-C3} to be about 7×10^{-13} ml molecule^{-1} s^{-1} at 295 K. Wilson, O'Donovan and Fristrom[18] give $k_{-C3} = 1.3 \times 10^{-11}$ ml molecule^{-1} s^{-1} at 1930 K. The listed rate coefficient, which corresponds to $k_{-C3} = 2 \times 10^{-11} \exp(-1000/T)$ ml molecule^{-1} s^{-1}, fits all these determinations, although the selected activation energy for the reaction (-C3) is larger than those given in Refs 16 and 17, and the listed expression would not be the best to use close to room temperature.

C4 Balaknin, Egorov and Intezarova[19] give $k_{-C4} = 2 \times 10^{-12} \exp(-2300/T)$ ml molecule^{-1} s^{-1} for $295 < T < 371$ K, Wong and Belles[20] give $k_{-C4} = 2 \times 10^{-11} \exp(-3600/T)$ ml molecule^{-1} s^{-1} for $356 < T < 628$ K and Brown and Smith[21] give $k_{-C4} = 2.5 \times 10^{-12} \exp(-2970/T)$ ml molecule^{-1} s^{-1} for $293 < T < 440$ K. At 360 K, these expressions yield 3.4×10^{-15} ml molecule^{-1} s^{-1}, 9×10^{-16} ml molecule^{-1} s^{-1} and 6.5×10^{-16} ml molecule^{-1} s^{-1} respectively and are therefore not in good agreement. We have selected $k_{-C4} = 5 \times 10^{-12} \exp(-3000/T)$ ml molecule^{-1} s^{-1} as a compromise, converting this to the listed value of k_{C4}.

C5 Directly measured values of k_{C5} do not agree well with one another: Jacobs, Giedt and Cohen[22] give $k_{C5} = 2 \times 10^{-11} \exp(-17600/T)$ ml molecule^{-1} s^{-1} but Blauer[23] gives $k_{C5} = 3 \times 10^{-12} \exp(-17500/T)$ ml molecule^{-1} s^{-1}; Kondratiev[32] summarizes measurements of k_{-C5} suggesting a pre-exponential factor in k_{C5} of about 4×10^{-11} ml molecule^{-1} s^{-1}. Values obtained for k_{-C5} at 300 K include 2.5×10^{-11} (Ref. 24), 1.8×10^{-11}

(Ref. 25), 6.3×10^{-11} (Ref. 26), 7×10^{-12} (Ref. 27) and 3×10^{-11} (Ref. 28) ml molecule^{-1} s^{-1}, and are thus also rather scattered. We have selected $k_{-C5} = 5.5 \times 10^{-11} \exp(-300/T)$ ml molecule^{-1} s^{-1} (2×10^{-11} ml molecule^{-1} s^{-1} at 300 K) as a compromise and converted this to $k_{C5} = 7 \times 10^{-11} \exp(-16500/T)$ ml molecule^{-1} s^{-1}. Further work on this reaction is clearly needed.

C6 Albright, Dodonov, Lavrovskaya, Morosov and Tal'rose[9] find $k_{C6} = 2 \times 10^{-10} \exp(-1200/T)$ ml molecule^{-1} s^{-1} for $294 \lesssim T \lesssim 565$ K. This expression gives $k_{C6} = 4 \times 10^{-12}$ ml molecule^{-1} s^{-1} at 300 K. Rabideau, Hecht and Lewis[27] give $k_{C6} = 4 \times 10^{-12}$ ml molecule^{-1} s^{-1} at 300 K, but Clyne, McKenney and Walker[24] give $k_{C6} = 2.5 \times 10^{-11}$ ml molecule^{-1} s^{-1} at this same temperature. We list $k_{C6} = 1 \times 10^{-10} \exp(-700/T)$ ml molecule^{-1} s^{-1} (1×10^{-11} ml molecule^{-1} s^{-1} at 300 K) as a compromise.

D1 This rate coefficient is estimated by comparison with those given for reactions D2 and D3 below.

D2 The listed value is based on measurements made by Polanyi[29] as long ago as 1932; no recent measurements have been reported. However, Kondratiev[30] discusses results of Taylor and Datz[31] which suggest that the rate coefficient of the reaction $K + HBr \rightarrow KBr + H$ is given by $k = 3 \times 10^{-12} T^{0.5} \exp(-1700/T)$ ml molecule^{-1} s^{-1}, or, at around 1600 K, by $k = 1.2 \times 10^{-10} \exp(-1700/T)$ ml molecule^{-1} s^{-1}. Other early results for this and other reactions reviewed by Kondratiev[32] suggest pre-exponential factors close to collision frequencies but activation energies which, in conjunction with the best modern values for the standard enthalpy changes of reaction D2 and others, imply unlikely negative activation energies for such reactions as the reverse of D2. The listed value for k_{D2} is a reasonable compromise. Taylor and Datz[31] used a molecular beam technique on a clean experimental system, but the early work suffers from uncertainties concerning the possible effects of condensed particles[29].

D3 This rate coefficient, like k_{D2}, is based on the work of Polanyi[29] and the review and discussion of Kondratiev[30,32].

D4 The listed value is estimated in a manner similar to that in which k_{D6} was obtained.

D5 The listed value is estimated in a manner similar to that in which k_{D6} was obtained.

D6 This rate coefficient is estimated on the basis of the general discussions of reactions of this type given by Jensen[33] and Sugden[34] and the experimental evidence of Jensen and Padley[35].

D7 The activation energy in k_{D7} is arbitrarily taken to be about 4 kJ mole^{-1} higher than the endothermicity[36]. The pre-exponential factor is estimated by analogy with those in k_{D3} and k_{D6}.

D8 The listed value is estimated in a manner similar to that in which k_{D7} was obtained, thermochemical data stemming from Refs 36 and 37.

D9 The listed value is estimated in a manner similar to that in which k_{D7} was obtained, thermochemical data stemming from Refs 36 and 38.

D10 The listed value is estimated in a manner similar to that in which k_{D7} was obtained.

D11 The listed value is estimated in a manner similar to that in which k_{D7} was obtained.

D12 The listed value is estimated in a manner similar to that in which k_{D6} was obtained.

E1 The following results have been obtained from shock tube measurements of k_{-E1} :

Reference	k_{-E1}, ml molecule^{-1} s^{-1}	k_{-E1} at 3500 K	k_{-E1} at 1500 K
39	$1.1 \times 10^{-11} \exp(-35000/T)$	5×10^{-16}	8×10^{-22}
40	$7 \times 10^{-11} \exp(-41000/T)$	6×10^{-16}	9×10^{-23}
41	$8 \times 10^{-11} \exp(-41600/T)$	6×10^{-16}	7×10^{-23}
42	$3.2 \times 10^{-13} T^{0.5} \exp(-35100/T)$	8×10^{-16}	9×10^{-22}

All the above values are for M ≡ Ar ; considerable disagreement exists concerning the relative efficiencies of Ar and HCl as M[41,43]. The results agree remarkably well at temperatures (≈ 3500 K) typical of the experiments but extrapolate to values in much less satisfactory agreement with one other at temperatures more typical of flames. Combined with the equilibrium constant, the results of Refs 39 and 42 give $k_{E1} \approx 7 \times 10^{-36} \exp(+17200/T)$ ml^2 molecule^{-2} s^{-1} , whilst those of Refs 40 and 41 give $k_{E1} \approx 5 \times 10^{-35} \exp(+10800/T)$ ml^2 molecule^{-2} s^{-1} . The surprisingly

steep temperature dependences of these values of k_{E1} may imply significant contributions from finite rate populations of vibrational levels of HCl, the kinetic importance of which might be lessened in the presence of molecular (as distinct from atomic) M . The absolute magnitude of k_{E1} at 3500 K implied by the results (1×10^{-33} ml^2 molecule^{-2} s^{-1} for M ≡ Ar) appears reasonable: that at 1500 K (> 1×10^{-31} ml^2 molecule^{-2} s^{-1}) less so. As an arbitrary compromise, we have selected $k_{E1} = 4 \times 10^{-26}$ T^{-2} ml^2 molecule^{-2} s^{-1} for a typical flame third body. Further work on this reaction remains necessary.

E2 Lloyd[44], on the basis of data from several sources, recommends $k_{E2} = 6 \times 10^{-34}$ exp(900/T) ml^2 molecule^{-2} s^{-1} for M ≡ Ar and 200 < T < 500 K . With the equilibrium constant given by $K_{E2} = 3 \times 10^{-25}$ exp(28600/T) ml molecule^{-1} , this would correspond approximately to $k_{-E2} = 2 \times 10^{-9}$ exp(-27700/T) ml molecule^{-1} s^{-1} ($k_{-E2} = 2 \times 10^{-24}$ ml molecule^{-1} s^{-1} at 800 K and 1.9×10^{-15} ml molecule^{-1} s^{-1} at 2000 K). Such values of k_{-E2} do not agree particularly well with direct measurements. Jacobs and Giedt[45] and Carabetta and Palmer[46], for example, give $k_{-E2} = 1.5 \times 10^{-10}$ exp(-24200/T) ml molecule^{-1} s^{-1} (1.1×10^{-23} ml molecule^{-1} s^{-1} at 800 K; 8.3×10^{-16} ml molecule^{-1} s^{-1} at 2000 K); Hiraoka and Hardwick[47] give $k_{-E2} = 1.5 \times 10^{-3}$ T$^{-1.5}$ exp(-28600/T) ml molecule^{-1} s^{-1} (1.9×10^{-23} ml molecule^{-1} s^{-1} at 800 K; 1.0×10^{-14} ml molecule^{-1} s^{-1} at 2000 K). Because of the scatter in the direct measurements of k_{-E2} and the fact that the k_{E2} value of Lloyd[44] implies one of k_{-E2} which lies between the direct values of the latter at 2000 K, we have accepted $k_{E2} = 6 \times 10^{-34}$ exp(900/T) ml^2 molecule^{-2} s^{-1} for M ≡ Ar and arbitrarily raised this through a factor of 3 to allow for the fact that typical flame collision partners M are probably amongst the more effective for both forward and backward steps of reaction E2.

E3 For M ≡ Ar , Jacobs, Giedt and Cohen[22] give $k_{-E3} = 1.9 \times 10^{-5}$ T^{-1} exp(-67500/T) ml molecule^{-1} s^{-1} and Blauer[23] gives $k_{-E3} = 8 \times 10^{-6}$ T^{-1} exp(-67500/T) ml molecule^{-1} s^{-1} . These data suggest $k_{E3} \approx 1 \times 10^{-29}$ T^{-1} ml^2 molecule^{-2} s^{-1} . Making allowance for the presence in flames of collision partners more efficient in inducing recombination than Ar , we suggest $k_{E3} = 3 \times 10^{-29}$ T^{-1} ml^2 molecule^{-2} s^{-1} . The measured values of k_{-E3} agree well with predictions of k_{E3} based on the theory of Benson and Fueno[48].

E4 Lloyd[44] recommends $k_{-E4} = 8 \times 10^{-12} \exp(-14300/T)$ ml molecule^{-1} s^{-1} for M ≡ Ar , weighting the work of Britton, Johnson and Seery[49,50] more heavily than that of Diesen[51,52]. In combination with the equilibrium constant, this gives $k_{E4} = 1 \times 10^{-36} \exp(4000/T)$ ml^2 molecule^{-2} s^{-1} , or $k_{E4} = 1.4 \times 10^{-35}$ ml^2 molecule^{-2} s^{-1} at 1500 K. Breshears and Bird[53] find $k_{-E4} = 6 \times 10^{-11} \exp(-17470/T)$ ml molecule^{-1} s^{-1} for M ≡ Ar (corresponding to $k_{E4} = 8 \times 10^{-36} \exp(850/T)$ ml^2 molecule^{-2} s^{-1} , or 1.4×10^{-35} ml^2 molecule^{-2} s^{-1} at 1500 K) and $k_{-E4} = 1.6 \times 10^{-10} \exp(-17520/T)$ ml molecule^{-1} s^{-1} for M ≡ F_2 ($k_{E4} = 2.1 \times 10^{-35} \exp(800/T)$ ml^2 molecule^{-2} s^{-1} , or 3.6×10^{-35} ml^2 molecule^{-2} s^{-1} at 1500 K). These results contrast rather sharply with Lloyd's suggestion[44] of $k_{E4} \approx 3 \times 10^{-34}$ ml^2 molecule^{-2} s^{-1} for 1000 < T < 2000 K , based upon the direct measurements of k_{-E4} and the theoretical estimates of k_{E4} made by Benson and Fueno[48]: the discrepancy may reflect deviations from the rate quotient law and uncertainties in the formulation of the equilibrium constant at high temperatures[44]. Ganguli and Kaufman[54] have reported $k_{E4} = 8 \times 10^{-35}$ ml^2 molecule^{-2} s^{-1} at 295 K for M ≡ Ar and Ultree[55] has found $k_{E4} = 6 \times 10^{-34}$ ml^2 molecule^{-2} s^{-1} at room temperature for M ≡ He . We suggest $k_{E4} = 1 \times 10^{-30} T^{-1.5}$ ml^2 molecule^{-2} s^{-1} (1.9×10^{-34} ml^2 molecule^{-2} s^{-1} at 300 K; 1.7×10^{-35} ml^2 molecule^{-2} s^{-1} at 1500 K) for use with M ≡ Ar , and convert this to $k_{E4} = 3 \times 10^{-30} T^{-1.5}$ ml^2 molecule^{-2} s^{-1} for a general flame third body.

F1 The theoretical arguments of Refs 33 and 34 and the experimental results of Bulewicz and Sugden[56] are a source of approximate values of k_{F1} and k_{-F1} . This work suggests that the pre-exponential factor in the rate coefficient of the reaction CuOH + M → Cu + OH + M cannot be much smaller than $6 \times 10^{-4} T^{-1}$ ml molecule^{-1} s^{-1} and, by analogy, the pre-exponential factor in k_{-F1} is probably not much less than this. If the activation energy in k_{-F1} is set equal to the endothermicity[36], $k_{-F1} K_{F1} = k_{F1}$ becomes not much less than $8 \times 10^{-28} T^{-1}$ ml^2 molecule^{-2} s^{-1} . A value of $3 \times 10^{-28} T^{-1}$ is suggested for use in flame calculations. This rate coefficient - greater than k_{A4} , but by no means the largest rate coefficient for a termolecular recombination of small neutral species ever suggested (cf. Ref. 57) - carries an uncertainty factor of one to two orders of magnitude. It is unlikely that the reaction is bimolecular rather than termolecular under flame conditions.

F2 The listed value is estimated in a manner similar to that in which k_{F1} was obtained.

F3 The listed value is estimated in a manner similar to that in which k_{F1} was obtained.

F4 The value of k_{F4}, like that of k_{F5}, is based on the review of Troe and Wagner[179].

F5 Troe and Wagner[179] suggest $k_{-F5} \approx 5 \times 10^{-9} \exp(-46000/T)$ ml molecule^{-1} s^{-1} for M ≡ Ar at around T = 3000 K, corresponding to $k_{F5} \approx 2 \times 10^{-32} \exp(2500/T)$ ml^2 molecule^{-2} s^{-1}. The value listed for a typical flame M seems reasonable by comparison.

F6 The value of k_{F6}, like that of k_{F5}, is based on the review of Troe and Wagner[179].

G1 Results of a number of flame determinations of k_{G1} are gathered together in Ref. 58. Recombination rate coefficients for $Me^+ + e^- + M \rightarrow Me + M$ all fit the expression $k = 4 \times 10^{-24} T^{-1}$ ml^2 molecule^{-2} s^{-1}, whatever the identity of the alkali metal atom Me, for any typical set of collision partners M. This recommendation is adopted as acceptably accurate for flame calculations.

G2 The listed value, like k_{G1}, is based on the recommendation of Ref. 58.

G3 The listed value, like k_{G1}, is based on the recommendation of Ref. 58.

G4 The listed value, like k_{G1}, is based on the recommendation of Ref. 58.

G5 Rate coefficients for k_{G5} and k_{-G5} have been measured by Kelly and Padley[157]. Their results suggest a value for k_{G5} at 2440 K of about 1×10^{-27} ml^2 molecule^{-2} s^{-1} and a T^{-2} temperature dependence for this rate coefficient. The listed value is based on this work.

H1 This value is taken from the recent work of Burdett and Hayhurst[59]. It stems from measurements made on atmospheric pressure flames of $H_2 + O_2 + N_2$ to which controlled amounts of lithium and chlorine are added. A mass spectrometric sampling method was used for flame temperatures between 1800 and 2400 K.

H2 This value is taken from the recent work of Burdett and Hayhurst[59]. It stems from measurements made on atmospheric pressure $H_2 + O_2 + N_2$ flames to which controlled amounts of sodium and chlorine are added. A mass spectrometric sampling method was used for flame temperatures between 1800 and 2400 K.

H3 The listed value is taken from Ref. 60.

H4 This rate coefficient is estimated by comparison with k_{H1}, k_{H2} and k_{H3}. The suggested value carries the implication that the potential energy curves for the different LiOH states are not unfavourably placed with respect to one another. The possible error bounds are consequently large. The pre-exponential factor in k_{-H4} implied is about 3×10^{-11} ml molecule^{-1} s^{-1} at 2000 K.

H5 This rate coefficient is estimated in a manner similar to that in which k_{H4} was obtained.

H6 This rate coefficient is estimated in a manner similar to that in which k_{H4} was obtained.

H7 Burdett and Hayhurst[59], from their mass spectrometric study of atmospheric pressure $H_2 + O_2 + N_2$ flames to which lithium and chlorine are added, find $k_{-H7} = 4 \times 10^{7}\ T^{-3.5} \exp(-77500/T)$ ml molecule^{-1} s^{-1}. This corresponds to $k_{H7} = 1.2 \times 10^{-15}\ T^{-3.5} \exp(-300/T)$ ml^2 molecule^{-2} s^{-1}, which agrees satisfactorily with calculations made on the basis of the theory of Bates and Flannery[61]. See also the notes on reactions H8 and H9.

H8 From the theory of Ref. 61 and polarisability and collision data of Ref. 62, the following values of k_{H8} for different collision partners M may be calculated:

M	k_{H8}, ml^2 molecule^{-2} s^{-1}		
	1000 K	2000 K	3000 K
N_2	3.6×10^{-27}	5.5×10^{-28}	1.9×10^{-28}
H_2O	7.8×10^{-27}	7.5×10^{-28}	2.0×10^{-28}
HCl	6.5×10^{-27}	7.5×10^{-28}	2.4×10^{-28}
CO	3.9×10^{-27}	6.8×10^{-28}	1.9×10^{-28}
CO_2	4.7×10^{-27}	7.2×10^{-28}	2.5×10^{-28}
O_2	3.5×10^{-27}	5.4×10^{-28}	1.9×10^{-28}

From their mass spectrometric measurements on atmospheric pressure flames at temperatures between 1800 and 2400 K to which sodium and chlorine are added, Burdett and Hayhurst[59] find $k_{-H8} = 1.1 \times 10^{7}\ T^{-3.5} \exp(-66750/T)$ ml molecule^{-1} s^{-1}. Translated into $k_{H8} = 5.5 \times 10^{-16}\ T^{-3.5} \exp(-750/T)$ ml^2

molecule^{-2} s^{-1} , this gives $k_{H8} = 8.2 \times 10^{-27}$ ml^2 molecule^{-2} s^{-1} at 1000 K, 1.07×10^{-27} ml^2 molecule^{-2} s^{-1} at 2000 K and 2.9×10^{-28} ml^2 molecule^{-2} s^{-1} at 3000 K. This agreement between theory and experiment is good. The value of Ref. 59 is adopted for flame calculations. It is noteworthy that the theory[61] predicts approximately the same values for the rate coefficients of $Cs^+ + F^- + M \rightleftharpoons CsF + M$ as are measured in shock tube experiments[63], although the theoretical and experimental temperature-dependences differ for this reaction. See also the note on reaction H9.

H9 From the theory of Ref. 61 and the polarisability and collision data of Ref. 62, the following values of k_{H9} for different collision partners M may be calculated:

M	k_{H9} , ml^2 molecule^{-2} s^{-1}		
	1000 K	2000 K	3000 K
N_2	4.2×10^{-27}	5.6×10^{-28}	1.6×10^{-28}
H_2O	1.0×10^{-26}	8.4×10^{-28}	2.5×10^{-28}
HCl	4.5×10^{-27}	8.1×10^{-28}	2.4×10^{-28}
CO	4.5×10^{-27}	5.9×10^{-28}	1.9×10^{-28}
CO_2	5.3×10^{-27}	7.4×10^{-28}	2.4×10^{-28}
O_2	4.1×10^{-27}	5.5×10^{-28}	1.8×10^{-28}

Burdett and Hayhurst[60] find $k_{-H9} = 2.2 \times 10^7\ T^{-3.5} \exp(-60800/T)$ ml molecule^{-1} s^{-1} , corresponding to $k_{H9} = 1.6 \times 10^{-15}\ T^{-3.5} \exp(-2400/T)$ ml^2 molecule^{-2} s^{-1} (4.6×10^{-27} , 1.3×10^{-27} and 4.9×10^{-28} ml^2 molecule^{-2} s^{-1} at 1000, 2000 and 3000 K respectively, and in good agreement with the theory). This value is adopted. The recommended values of k_{-F4} , k_{-F5} , k_{-F6} and k_{-H7} , k_{-H8} and k_{-H9} are broadly in line with the relative probabilities for collisional dissociation of the alkali halides AB into $A^+ + B^-$ and A + B respectively discussed in Ref. 179. See also the notes on reaction H8.

J1 This rate coefficient is estimated by comparison with k_{J2} and k_{J10} , no experimental measurements of k_{J1} being available.

J2 Mandl[64] has measured k_{-J2} in shock tube experiments for the temperature range 3500-5500 K. He finds that $k_{-J2} = 1 \times 10^{-10} \exp(-42000/T)$ ml

molecule^{-1} s^{-1} for M ≡ Ar or N_2 . This corresponds to a value for $k_{J2} \approx 1 \times 10^{-32}$ exp(3000/T) ml^2 molecule^{-2} s^{-1} , which is adopted.

J3 Measurements of this rate coefficient have produced widely scattered results (cf. Refs 65-72). Fehsenfeld, Ferguson and Schmeltekopf[68,69] and Howard, Fehsenfeld and McFarland[65] have measured k_{-J3} as 1.0×10^{-9} ml molecule^{-1} s^{-1} at around room temperature. This would suggest a value of k_{-J3} of at least 1×10^{-10} ml molecule^{-1} s^{-1} at flame temperatures ≈2000 K [73] and imply a pre-exponential factor in k_{J3} well in excess of 10^{-8} ml molecule^{-1} s^{-1} . The preliminary results of Buchelnikova[71], on the other hand, are interpreted by Calcote and Jensen[70] as implying a pre-exponential factor in k_{J3} orders of magnitude lower. In an attempt to resolve this discrepancy, Burdett and Hayhurst[66,67] have studied the reaction in the gases sampled from $H_2 + O_2 + N_2$ flames containing Cl^-. They conclude that reaction J3 is balanced at atmospheric pressure in flames of temperatures 1800-2800 K, but interpret their results in terms of relaxation of the equilibrium within the mass spectrometric sampling cone used, finding $k_{-J3} = 7 \times 10^{-10}$ ml molecule^{-1} s^{-1} . This agrees with the values of Refs 65, 68 and 69. In contrast, Calcote[72] reports that Miller and Gould find $k_{J3} = 3 \times 10^{-10}$ exp(-13000/T) ml molecule^{-1} s^{-1}; these authors also sampled atmospheric pressure $H_2 + N_2 + O_2$ flames containing Cl^- with a mass spectrometer, but interpreted their results in terms of non-equilibrium in the flame itself. Miller and Gould's value for k_{J3} corresponds to $k_{-J3} \approx 10^{-13}$ ml molecule^{-1} s^{-1} , a result more consistent with that of Buchelnikova[71]. Because Burdett and Hayhurst[67] explain how sampled profiles of $[Cl^-]$ in flames might falsely suggest that reaction J3 is not balanced in the flames themselves, we accept their value as the best currently available, but recommend that still further work on the reaction is needed. The k_{-J3} value of 7×10^{-10} ml molecule^{-1} s^{-1} (independent of temperature for 1800 < T < 2800 K) corresponds to $k_{J3} = 1.4 \times 10^{-7}$ exp(-7600/T) ml molecule^{-1} s^{-1} .

J4 Miller and Gould[74] have made measurements on dissociative attachment of electrons to HBO_2 in $H_2 + O_2 + N_2$ flames at temperatures between 1730 and 2250 K and pressures of 13 to 101 kN m^{-2} (0.13-1 atmosphere). They interpret their results in terms of a value for k_{J4} of 3×10^{-10} exp(-11000/T) ml molecule^{-1} s^{-1} , the pre-exponential factor in k_{J4} being similar to that in k_{J3} found by the same workers[72]. It is possible, however, that these results might alternatively be interpreted in terms of reaction J4

being balanced in the flame gases but unbalanced to varying extents in the mass spectrometer sampling system used (cf. Ref. 67). Following the arguments of Ref. 67, we suggest using $k_{J4} = 1 \times 10^{-8} \exp(-11000/T)$ ml molecule^{-1} s^{-1} for the present. Such a value carries wide error bounds, and further study of this reaction is necessary.

J5 This rate coefficient is estimated by comparison with k_{J3}, k_{J4} and k_{J7} (see the notes on these rate coefficients). The uncertainty factor is consequently large.

J6 This rate coefficient is estimated in a manner similar to that in which k_{J5} was obtained.

J7 The rate coefficient k_{-J7} has been measured at around room temperature by Ferguson, Fehsenfeld and Schmeltekopf[69] as about 1×10^{-9} ml molecule^{-1} s^{-1}. The temperature dependence of k_{-J7} is probably slight, but might be expected to decrease this value of k_{-J7} to not less than 10^{-10} ml molecule^{-1} s^{-1} at typical flame temperatures[73]. With JANAF data[36] for OH^-, this leads to a value of k_{J7} of about $1 \times 10^{-7} \exp(-35000/T)$ ml molecule^{-1} s^{-1} - i.e. to a pre-exponential factor in k_{J7} of similar magnitude to that found in k_{J3} by Burdett and Hayhurst[66,67]. Calcote and Jensen[70], on the other hand, interpret the preliminary results of Buchelnikova[71] as indicating a pre-exponential factor in k_{J7} of not more than 10^{-10} ml molecule^{-1} s^{-1}. The listed value is a compromise which weights the results of Ref. 69 more strongly than those of Ref. 71.

J8 This rate coefficient is estimated by comparison with other ion/molecule reaction rate coefficients given in, e.g., Ref. 75. Thermochemical data for the reaction stem from Ref. 38.

J9 This rate coefficient is estimated by comparison with other ion/molecule reaction rate coefficients given in, e.g., Ref. 75. Thermochemical data for the reaction stem from Ref. 37.

J10 This value is based on the work of Pack and Phelps[76,77]. It should be within a factor of 30 of the true value under flame conditions.

L1 This rate coefficient is estimated by comparison with k_{L2} and k_{L3}. The endothermicity measured by Hayhurst[78] is preferred to that given by Dzidic and Kebarle[79] because the latter is based upon a rather inaccurate extrapolation of results for higher hydrates of Li^+.

L2 Johnsen, Brown and Biondi[80] find that, at 300 K, $k_{-L2} = 1 \times 10^{-28}$ and 4.7×10^{-30} ml^2 $molecule^{-2}$ s^{-1} for $M \equiv H_2O$ and He respectively. If k_{-L2} is assumed to vary as T^{-1} (a reasonable but arbitrary and uncertain assumption), these values may be converted to 1.5×10^{-29} ml^2 $molecule^{-2}$ s^{-1} (H_2O) and 7×10^{-31} ml^2 $molecule^{-2}$ s^{-1} (He) at 2000 K. In combination with the equilibrium constant, these results yield $k_{L2} = 1.5 \times 10^{-6}$ exp(-15000/T) and 7×10^{-8} exp(-15000/T) ml $molecule^{-1}$ s^{-1} respectively. We suggest adopting $k_{L2} = 3 \times 10^{-7}$ exp(-15000/T) for use in flame calculations. For reactions L1-L3, the possibility of deviations from the rate quotient law, and perhaps even contributions from bimolecular hydration under some conditions, add to the uncertainties involved.

L3 Johnsen, Brown and Biondi[80] give $k_{-L3} = 4.5 \times 10^{-29}$ ml^2 $molecule^{-2}$ s^{-1} for $M \equiv H_2O$ and $k_{-L3} = 2.6 \times 10^{-30}$ ml^2 $molecule^{-2}$ s^{-1} for $M \equiv$ He at 300 K. With k_{-L3} arbitrarily assumed to vary as T^{-1}, these values convert to 7×10^{-30} ml^2 $molecule^{-2}$ s^{-1} (H_2O) and 4×10^{-31} ml^2 $molecule^{-2}$ s^{-1} (He) at 2000 K, and, combined with the equilibrium constant, give $k_{L3} = 3 \times 10^{-7}$ exp(-10000/T) ml $molecule^{-1}$ s^{-1} and $k_{L3} = 2 \times 10^{-8}$ exp(-10000/T) ml $molecule^{-1}$ s^{-1} respectively. We suggest adopting $k_{L3} = 1 \times 10^{-7}$ exp(-10000/T) ml $molecule^{-1}$ s^{-1} for use in flame calculations. See also the note on reaction L2.

L4 This rate coefficient is estimated by comparison with coefficients for other dissociative recombinations of positive ions with electrons, including the fairly reliable values for k_{T11}, k_{S1} and k_{S25} (see Refs 82-88). It is emphasized that the products of such dissociative recombinations are rarely identified, and one must be wary of the apparent implications of a given dissociative recombination rate coefficient for the reverse (chemi-ionization) step. See also the note on reaction L1.

L5 This rate coefficient is estimated in a manner similar to that in which k_{L4} was obtained.

L6 This rate coefficient is estimated in a manner similar to that in which k_{L4} was obtained.

L7 Burdett, Hayhurst and Morley[89] have obtained a value for the rate coefficient of $H_3O^+ + Cl^- \rightarrow H_2O + HCl$ of about 4×10^{-8} ml $molecule^{-1}$ s^{-1} in the temperature range 1800-2600 K. The reaction products were not identified. It seems reasonable to assign a similar value to k_{L7}. The

enthalpy change of reaction L7 implied by the work of Hayhurst[78] is preferred to that corresponding to the work of Dzidic and Kebarle[79] for the reason given in the notes on reaction L1. Great caution must be exercised in considering the implications of k_{L7} for the reverse (chemi-ionization) step because the products of the reaction are uncertain.

L8 This rate coefficient is estimated in a manner similar to that in which k_{L7} was obtained.

L9 This rate coefficient is estimated in a manner similar to that in which k_{L7} was obtained.

L10 This rate coefficient is estimated in a manner similar to that in which k_{L7} was obtained.

L11 This rate coefficient is estimated in a manner similar to that in which k_{L7} was obtained.

L12 This rate coefficient is estimated in a manner similar to that in which k_{L7} was obtained.

M1 We are aware of no experimental measurements of k_{M1}. The listed value is estimated by comparison with three body recombination rate coefficients for which data are available, including k_{A1} and k_{E2}.

M2 The pre-exponential factor in k_{M2} is thought likely to be close to the collision frequency. An arbitrary activation energy of 12 kJ $mole^{-1}$ is inserted into the listed expression for k_{M2} as a result of comparison of reaction M2 with other, formally similar, bimolecular reactions.

M3 This rate coefficient is estimated in a manner similar to that in which k_{M2} was obtained.

M4 This rate coefficient is estimated in a manner similar to that in which k_{M2} was obtained.

M5 Clyne and Walker[90] have obtained a lower limit for k_{M5} at 300 K of 1×10^{-11} ml $molecule^{-1}$ s^{-1}. The listed rate coefficient is consistent with this and appears reasonable by comparison with rate coefficients in groups B and C. Note, however, that the reaction $ClO + H_2 \rightarrow HCl + OH$ is apparently very slow at room temperature[91].

M6 Watson[92] recommends $k_{M6} = 5 \times 10^{-11}$ ml $molecule^{-1}$ s^{-1} at 300 K, implying that the activation energy cannot be large. Clyne and Nip[93] have recently

reported $k_{M6} = 1.1 \times 10^{-10} \exp(-220/T)$ ml molecule^{-1} s^{-1} , with a very low activation energy indeed. Clyne and Nip's value is adopted.

M7 Cox and Derwent[94] argue that k_{-M7} must be lower than k_{P2} at 306 K; for k_{P2} they give a value of 2.5×10^{-11} ml molecule^{-1} s^{-1} at this temperature. We have listed $k_{P2} = 1.2 \times 10^{-10} \exp(-480/T)$ ml molecule^{-1} s^{-1} . If k_{-M7} , in line with Cox and Derwent's argument, is set equal to $1 \times 10^{-10} \exp(-1000/T)$ ml molecule^{-1} s^{-1} (4×10^{-12} ml molecule^{-1} s^{-1} at 306 K), k_{M7} becomes $1.3 \times 10^{-11} \exp(-1380/T)$ ml molecule^{-1} s^{-1} , the listed value.

N1 This rate coefficient is estimated by comparison with k_{N2} and k_{N3} . We are not aware of any experimental data, kinetic or thermochemical, for this reaction.

N2 This value stems from the work of Carabetta and Kaskan[95,96]. The T^{-1} temperature dependence is arbitrarily inserted: Carabetta and Kaskan observed little variation of k_{N2} with temperature. The enthalpy change for the reaction is given by McEwan and Phillips[97].

N3 This rate coefficient is based on the work of Carabetta and Kaskan[95,96]. See also the note to reaction N2. The equilibrium constant is estimated on the basis of results given in Ref. 97.

N4 This rate coefficient is estimated by comparison with k_{P4} . See also the note on reaction N1.

N5 This rate coefficient is estimated by comparison with k_{P4} .

N6 This rate coefficient is estimated by comparison with k_{P4} . See also the note on reaction N3.

N7 This rate coefficient is estimated by comparison with k_{P5} . See also the note on reaction N1.

N8 This rate coefficient is estimated by comparison with k_{P5} .

N9 This rate coefficient is estimated by comparison with k_{P5} . See also the note on reaction N3.

N10 The listed rate coefficient is estimated by comparison with k_{P8} , which is itself an estimated value. See also the note on reaction N1.

N11 This rate coefficient is estimated in a manner similar to that in which k_{N10} was obtained.

N12 This rate coefficient is estimated in a manner similar to that in which k_{N10} was obtained. See also the note on reaction N3.

N13 Padley and Sugden[98] give $k_{N13} = 6 \times 10^{-32}$ ml^2 molecule^{-2} s^{-1} at flame temperatures $\approx$2000 K. If the improved quenching data recommended by Jenkins[99] are used to re-interpret these results, a slightly higher value of k_{N13} is obtained. That selected is as good an estimate as is currently available.

N14 This rate coefficient is based on the work of Refs 98 and 99. See also the note on reaction N13.

N15 Padley and Sugden[98] give $k_{N15} = 2 \times 10^{-32}$ ml^2 molecule^{-2} s^{-1} at flame temperatures $\approx$2000 K. With improved quenching data[99], this is converted to $k_{N15} = 6 \times 10^{-32}$ ml^2 molecule^{-2} s^{-1} . Carabetta and Kaskan[100] find $k_{N15} = 4 \times 10^{-31}$ ml^2 molecule^{-2} s^{-1} , which Jenkins[99] suggests may be a little too high. The selected value seems a reasonable compromise.

N16 This rate coefficient is based on the work described in Refs 98-100. See also the note on reaction N15.

N17 This value is based on the work of Carabetta and Kaskan[100], corrected for the improved quenching cross sections given by Jenkins[99].

N18 This value is based on the work of Carabetta and Kaskan[100], corrected for the improved quenching cross sections given by Jenkins[99].

N19 Quenching cross sections for the Na $^2P_{1/2}$ and $^2P_{3/2}$ states in collisions with different molecules (σ^2 , not $\pi\sigma^2$) are given by Jenkins[101] as follows:

Molecule	Cross section (10^{-16} cm^2)
H_2	2.87
N_2	6.95
O_2	12.3
CO_2	17.0
H_2O	0.5
CO	11.9

These results are reasonably consistent with previous values[101]. For a typical flame molecule of molecular weight 25 amu and reduced mass 2×10^{-23} g , it is reasonable to take a quenching cross section σ^2 of

10×10^{-16} cm^2 . The value of k_{-N19} is then 1.2×10^{-11} $T^{0.5}$ ml molecule^{-1} s^{-1} ; this translates into the value of k_{N19} listed.

N20 This rate coefficient was obtained in the same way as k_{N19} .

N24 Jenkins[102], Burhop and Massey[103] and Krause[104] all consider the cross section of reaction N24 to be large and the value of k_{N24} to be close to the collision frequency. The value listed should not be greatly in error.

N25 This rate coefficient is set equal to that of the analogous reaction for sodium, N13.

N26 This rate coefficient is set equal to that of the analogous reaction for sodium, N14.

N27 This rate coefficient is set equal to that of the analogous reaction for sodium, N15.

N28 This rate coefficient is set equal to that of the analogous reaction for sodium, N16.

N29 This rate coefficient is set equal to that of the analogous reaction for sodium, N17.

N30 This rate coefficient is set equal to that of the analogous reaction for sodium, N18.

N31 Quenching cross sections for the K $^2P_{1/2}$ and $^2P_{3/2}$ states with different molecules (σ^2 , not $\pi\sigma^2$) are given by Jenkins[105] as follows:

Molecule	Cross section (10^{-16} cm^2)
H_2	1.03
CO_2	21.4
H_2O	0.9
N_2	5.6
O_2	15.5
CO	12.4

For a typical flame molecule, it is reasonable to take a cross section σ^2 of 10×10^{-16} cm^2 for a reduced mass of 2.5×10^{-23} g . The deactivation rate coefficient is then 1.2×10^{-11} $T^{+0.5}$ ml molecule^{-1} s^{-1} . This implies a value for k_{N31} of 1.2×10^{-11} $T^{0.5}$ exp(-18690/T) ml molecule^{-1} s^{-1} .

N32 This rate coefficient is obtained in the same way as k_{N31} .

N35 This rate coefficient is estimated in a manner similar to that in which k_{N24} was obtained.

N38 This rate coefficient is estimated by comparison with rate coefficients of group P reactions.

N41 This rate coefficient is estimated by comparison with those of group P reactions.

P1 Baulch, Drysdale, Horne and Lloyd[4] discuss this reaction in detail and recommend $k_{P1} = 4.1 \times 10^{-33} \exp(500/T)$ ml^2 molecule^{-2} s^{-1} for M ≡ He or Ar . For an "average" third body other than H_2O, it would seem reasonable to write $k_{P1} = 1 \times 10^{-32} \exp(500/T)$ ml^2 molecule^{-2} s^{-1} (see data for relative efficiencies of H_2 , CO_2 , O_2 , N_2 and inert gases summarized in Ref. 4). For M ≡ H_2O , however, the results collected in Ref. 4 suggest a value for k_{P1} as high as $1 \times 10^{-31} \exp(500/T)$ ml^2 molecule^{-2} s^{-1} . Under conditions where this reaction plays an important part, it might therefore be wise to describe reaction P1 in terms of two separate rates, one for M ≡ H_2O and one for M ≡ any other flame molecule . The listed value is intended for use in applications when both water and other molecules are present. The rather wide uncertainty limits thus do not do justice to the accuracy of the experimental data, as they stem largely from the fact that allowance is made for variations of H_2O mole fractions from one flame to another.

P2 Cox and Derwent[94] give a value for k_{P2} of 2.5×10^{-11} ml molecule^{-1} s^{-1} at 306 K. The activation energy must therefore be small. We have arbitrarily inserted an activation energy of 4 kJ mole^{-1}, obtaining the listed value of k_{P2} .

P3 This recommendation is taken from Refs 4 and 106.

P4 This recommendation is taken from Refs 4 and 106.

P5 Baulch, Drysdale, Horne and Lloyd[4] and Lloyd[106] recommend a rate coefficient of $1.2 \times 10^{-12} \exp(-9400/T)$ ml molecule^{-1} s^{-1} for the reaction $H_2 + HO_2 \rightarrow H_2O_2 + H$, the products of this reaction being preferred to $H_2O + OH$ [4]. In flame calculations, however, the main interest in such a reaction is usually in its rate of removal of HO_2 rather than in its products. We disregard H_2O_2 as a result of its relative unimportance as a reaction

intermediate in high temperature flames. Reaction P5 as written should account adequately for removal of HO_2 by H_2 in these flames.

P6 The value listed is that suggested by Baulch, Drysdale, Duxbury and Grant[3]. It differs substantially from that of Ref. 1 at the lower temperatures of interest; this reaction has attracted a good deal of attention since 1971, partly because it is thought to play an important part in removing CO from polluted air[3].

P7 Lloyd[106] estimates $k_{P7} = 8 \times 10^{-11} \exp(-500/T)$ ml molecule^{-1} s^{-1} , which seems as reasonable a value as any.

P8 Hochanadel, Ghormley and Ogren[107] and DeMore and Tschuikow-Roux[108] suggest $k_{P8} = 2 \times 10^{-10}$ ml molecule^{-1} s^{-1} at 300 K, implying a very small activation energy; Lloyd[106] lists $k_{P8} = 8 \times 10^{-11} \exp(-500/T)$ ml molecule^{-1} s^{-1} . We suggest using a temperature-independent value of 1×10^{-10} ml molecule^{-1} s^{-1} for flame calculations.

Q1 Baulch, Drysdale, Duxbury and Grant[3] decline to make a recommendation for k_{Q1} because no experimental measurements are available. The listed value is estimated by comparison with k_{Q4} , consistent with the result of Mack and Thrush[109] that $k_{Q1} \approx 0.14\ k_{Q4}$ at 300 K.

Q2 Baulch, Drysdale, Duxbury and Grant[3] decline to make a recommendation for k_{Q2} because no experimental measurements are available. The rough estimate of Ref. 1 is retained.

Q3 Baulch, Drysdale, Duxbury and Grant[3] suggest $k_{Q3} = 2 \times 10^{-33} \exp(-850/T)$ ml^2 molecule^{-2} s^{-1} for $M \equiv H_2$ in the temperature range 300-770 K. We adopt this expression for use in flames for all M . The large uncertainty bounds reflect doubts concerning the temperature-dependence of k_{Q3} and its possible variation with the nature of M .

Q4 Baulch, Drysdale, Duxbury and Grant[3] decline to make a recommendation for k_{Q4} because of the lack of experimental data. Brennen, Gay, Glass and Niki[110] consider k_{Q4} to be greater than k_{Q9} . The listed estimate is consistent with this view.

Q5 Although there has been a good deal of work on this reaction, it is not easy to select a best value for the rate coefficient. Schofield[111] and Kondratiev[32] recommend $k_{Q5} = 7 \times 10^{-11} \exp(-5800/T)$ and $9 \times 10^{-11} \exp(-6450/T)$ ml molecule^{-1} s^{-1} respectively, but Fristrom and Westenberg[6],

taking a different view of the relative reliabilities of the same experimental data, give $k_{Q5} = 8 \times 10^{-10} \exp(-6750/T)$ ml molecule^{-1} s^{-1}. More recently, a theoretical analysis by Clark and Dove[112] has suggested $k_{Q5} = 3.7 \times 10^{-20} T^3 \exp(-4400/T)$ ml molecule^{-1} s^{-1}. We suggest $k_{Q5} = 7 \times 10^{-10} \exp(-7500/T)$ ml molecule^{-1} s^{-1} as a compromise for use in flame calculations.

Q6 Schofield[111], Kondratiev[32] and Herron and Huie[113] recommend $k_{Q6} = 5 \times 10^{-11} \exp(-4000/T)$, $8 \times 10^{-11} \exp(-4500/T)$ and $3.5 \times 10^{-11} \exp(-4550/T)$ ml molecule^{-1} s^{-1} respectively, on the basis of data from several sources. The listed value agrees well with these recommendations, although rather less well with Brabbs and Brokaw's determination[114] of $k_{Q6} = 3 \times 10^{-10} \exp(-5900/T)$ ml molecule^{-1} s^{-1}, for the temperature range of interest.

Q7 This rate coefficient is based on the recommendation of Wilson and Westenberg[115]. It agrees well with the expressions $k_{Q7} = 1.2 \times 10^{-10} \exp(-3000/T)$ ml molecule^{-1} s^{-1} and $k_{Q7} = 1.3 \times 10^{-10} \exp(-2900/T)$ ml molecule^{-1} s^{-1} suggested by Schofield[111] and Kondratiev[32] respectively and with other results summarized in Ref. 116.

Q8 Morris and Niki[117] find $k_{Q6} = 1.4 \times 10^{-11}$ ml molecule^{-1} s^{-1} at 300 K. Wilson[118] suggests $k_{Q8} = 8 \times 10^{-11}$ ml molecule^{-1} s^{-1} for $300 < T < 1600$ K. Peeters and Mahnen[119] give $k_{Q8} = 3.8 \times 10^{-11}$ ml molecule^{-1} s^{-1} for $1400 < T < 1800$ K, whilst Kondratiev[32] tentatively suggests $k_{Q8} = 1 \times 10^{-10}$ ml molecule^{-1} s^{-1} for $770 < T < 1500$ K. All these values are much higher than the early value of Avramenko and Lorentzo[120]. The listed value is a compromise.

Q9 Schofield[111] gives a value for k_{Q9} of $1 \times 10^{-10} \exp(-2300/T)$ ml molecule^{-1} s^{-1}. Kondratiev[32] suggests the similar expression $k_{Q9} = 5 \times 10^{-11} \exp(-2100/T)$ ml molecule^{-1} s^{-1}. The latter expression is adopted.

Q10 Kondratiev[32] suggests $k_{Q10} = 2 \times 10^{-10} \exp(-1700/T)$ ml molecule^{-1} s^{-1}. The value listed differs only slightly from this expression, but agrees better with results reported by Mack and Thrush[109].

Q11 Fenimore[121] suggests a bimolecular rate coefficient of 7×10^{-12} ml molecule^{-1} s^{-1} at 1970-2190 K for the reaction of CH_3 with OH. The products of reaction are uncertain, but may well be $CH_2O + H$. This value is listed, but must be applied with caution. The steps leading to production of CH_2O

from CH_3 in combustion processes are not well understood, and it is difficult to envisage the transition complex if reaction Q11 occurs as a single step. See also the notes on reaction Q13.

Q12 Fristrom and Westenberg[6] argue that reaction Q12, with a rate coefficient $\approx 10^{-13}$ ml molecule^{-1} s^{-1}, can be used to describe one path of conversion of CH_3 to CH_2O in combustion systems (see the notes on reaction Q13). Work on numerical matching of shock tube concentration profiles suggests $k_{Q12} = 2 \times 10^{-12} \exp(-6260/T)$ ml molecule^{-1} s^{-1} (Ref. 122) and $k_{Q12} = 3.3 \times 10^{-14}$ ml molecule^{-1} s^{-1} at 1350 K (Ref. 123). Similar analysis of shock-initiated methane oxidation[124] results in $k_{Q12} = 2 \times 10^{-13} \exp(-5000/T)$ ml molecule^{-1} s^{-1} at 1900-2400 K. This last expression gives $k_{Q12} = 5 \times 10^{-15}$ ml molecule^{-1} s^{-1} at 1350 K and therefore does not agree well with the results of Refs 122 and 123. Brabbs and Brokaw[114] argue against the occurrence of reaction Q12 in similar combustion regimes, suggesting instead $CH_3 + O_2 \rightarrow CH_3O + O$ followed by $CH_3O + M \rightarrow CH_2O + H + M$ or $CH_3O + CO \rightarrow CO_2 + CH_3$. Clearly this reaction is a controversial one. For the present, we suggest a compromise between the values of Refs 122 and 124, $5 \times 10^{-13} \exp(-5500/T)$ ml molecule^{-1} s^{-1}, with wide uncertainty bounds.

Q13 Fenimore and Jones[125] suggest reaction Q13 as a means of converting CH_3 to CH_2O in combustion systems, assigning k_{Q13} a value of 3×10^{-11} ml molecule^{-1} s^{-1} for $1200 < T < 1900$ K. Several other workers have also interpreted their results in terms of this reaction. Bowman[124] gives $k_{Q13} = 1.7 \times 10^{-10}$ ml molecule^{-1} s^{-1} at 1900-2400 K. Biordi, Lazzara and Papp[126] give $k_{Q13} = 1.8 \times 10^{-10}$ ml molecule^{-1} s^{-1} at 1550-1725 K. Izod, Kistiakowski and Matsuda[122] report $k_{Q13} = 6 \times 10^{-11} \exp(-1600/T)$ ml molecule^{-1} s^{-1} and Clark, Izod and Matsuda[123] give $k_{Q13} = 4 \times 10^{-11}$ ml molecule^{-1} s^{-1} at 1350 K. All these results are obtained via fitting of concentration profiles to rather complicated mechanisms, however, and Dixon-Lewis and Williams[127] argue that the results of Baldwin, Jackson, Walker and Webster[128] rule out significant contributions from reaction Q13 in premixed flames containing methane. Nevertheless, it seems probable (although not certain) that there is a rapid direct step from CH_3 to CH_2O which occurs in high temperature methane oxidation, and reaction Q13 is arbitrarily chosen as one means of accomplishing this conversion for the present. The value selected for the rate coefficient, $1 \times 10^{-10} \exp(-500/T)$ ml molecule^{-1} s^{-1}, is a compromise amongst the results of

Refs 122-126, and is in reasonable agreement with other values collected together in Ref. 116. The retention of reaction Q13 is thus analogous to that of reactions Q11 and Q12, objections to these last two reactions also having been raised (see, for example, Refs 115, 125, 127).

Q14 Dean and Kistiakowski[129] find that at 10 kPa pressure in shock tubes the decomposition $CH_4(+ M) \rightarrow CH_3 + H(+ M)$ follows bimolecular kinetics, and for $M \equiv Ar$ give $k_{-Q14} = 2.7 \times 10^{-6} \exp(-51500/T)$ ml molecule^{-1} s^{-1}. The work of Ref. 130 gives $k_{-Q14} = 4 \times 10^{-10} \exp(-32500/T)$ ml molecule^{-1} for $M \equiv$ inert gas, the activation energy in which is startlingly low. Bowman[124] gives $k_{-Q14} = 2.3 \times 10^{-7} \exp(-44500/T)$ ml molecule^{-1} s^{-1}, also for inert gas M. These three expressions yield:

	Ref. 129	Ref. 130	Ref. 124
k_{-Q14}, ml molecule^{-1} s^{-1}, 1500 K	3×10^{-21}	2×10^{-19}	3×10^{-20}
k_{-Q14}, ml molecule^{-1} s^{-1}, 2000 K	2×10^{-17}	4×10^{-17}	5×10^{-17}
k_{-Q14}, ml molecule^{-1} s^{-1}, 2500 K	3×10^{-15}	9×10^{-16}	4×10^{-15}

The rate coefficients thus agree fairly well for the typical experimental temperatures 2000-2500 K, but imply quite discordant values outside this temperature range. Direct measurements of k_{Q14} (e.g. Ref. 131) give values $\approx 3 \times 10^{-29}$ ml^2 molecule^{-2} s^{-1} at about 300 K, with only a slight dependence on temperature. We suggest $k_{Q14} = 8 \times 10^{-22} T^{-3}$ ml^2 molecule^{-2} s^{-1} for $1000 < T < 3000$ K for $M \equiv Ar$ (3×10^{-29} ml^2 molecule^{-2} s^{-1} at 300 K; 1×10^{-31} ml^2 molecule^{-2} s^{-1} at 2000 K). In the temperature range of interest, this corresponds to $k_{-Q14} = 2 \times 10^5 T^{-3} \exp(-54600/T)$ ml molecule^{-1} s^{-1}, giving $k_{-Q14} = 3.5 \times 10^{-17}$ ml molecule^{-1} s^{-1} at 2000 K and $k_{-Q14} = 4 \times 10^{-15}$ ml molecule^{-1} s^{-1} at 2500 K. For $M \equiv$ a typical flame molecule, we suggest the listed value of $2 \times 10^{-21} T^{-3}$ ml^2 molecule^{-2} s^{-1}. The discrepancies amongst the room temperature and shock tube measurements are both marked and unaccounted for, and the listed error bounds are therefore wide. The form of the equilibrium constant for reaction Q14 listed is particularly unsuitable for extrapolation to temperatures below 1000 K; quite different expressions for both this constant and k_{Q14} would be selected at low temperatures.

Q15 Benson and O'Neal[132] recommend $k_{-Q15} = 5.6 \times 10^{16} \exp(-45070/T)$ s^{-1}, which corresponds to $k_{Q15} = 5 \times 10^{-11} \exp(-1190/T)$ ml molecule^{-1} s^{-1}. At 293 K,

however, this gives $k_{Q15} = 9 \times 10^{-13}$ ml molecule^{-1} s^{-1} , which is considerably lower than has been measured directly (James and Simons[133], for example, give $k_{Q15} = 5.6 \times 10^{-11}$ ml molecule^{-1} s^{-1} at 293 K; Parkes, Paul and Quinn[134] give $k_{Q15} = 4 \times 10^{-11}$ ml molecule^{-1} s^{-1} for $250 < T < 450$ K). We suggest using $k_{Q15} = 1 \times 10^{-11} \exp(500/T)$ ml molecule^{-1} s^{-1} . This fits the low temperature results reasonably well, agrees adequately with the results reported in Ref. 135 for $1120 < T < 1400$ K , and yields an expression for k_{-Q15} , $1.1 \times 10^{16} \exp(-43380/T)$ s^{-1} , which is not too discordant with the collected, rather scattered, results summarized by Benson and O'Neal[132] or with more recent work (e.g. Ref. 136). The error bounds remain rather wide at the higher temperatures of flame interest.

Q16 Schofield[111] and Kondratiev[32], on the basis of data from several sources, suggest $k_{Q16} = 2.2 \times 10^{-10} \exp(-5200/T)$ and $k_{Q16} = 1.7 \times 10^{-10} \exp(-4800/T)$ ml molecule^{-1} s^{-1} respectively. Clarke and Dove[112], however, suggest $k_{Q16} = 9 \times 10^{-22} T^{3.5} \exp(-2620/T)$ ml molecule^{-1} s^{-1} as being more acceptable on theoretical grounds. These three expressions agree reasonably well for the temperatures of 500-1000 K at which most of the experimental measurements have been made, but the recommendation of Clarke and Dove[112] gives markedly greater values at higher temperatures. We suggest using $k_{Q16} = 5 \times 10^{-17} T^2 \exp(-3500/T)$ ml molecule^{-1} s^{-1} for the temperature range of interest.

Q17 Halstead, Leathard, Marshall and Purnell[137] suggest $k_{Q17} = 8 \times 10^{-11}$ ml molecule^{-1} s^{-1} on the basis of their measurements at 290 K and 8-16 torr. The products of reaction here are in some doubt, and may be $CH_3 + CH_3$ rather than $C_2H_4 + H_2$. The activation energy is likely to be small, and a temperature-independent value of 8×10^{-11} ml molecule^{-1} s^{-1} is listed, with wide error bounds.

Q18 The suggestion of Schofield[111] that $k_{Q18} = 2.9 \times 10^{-11} \exp(-3460/T)$ ml molecule^{-1} s^{-1} is adopted.

Q19 Benson and Haugen[138] suggest $k_{Q19} = 7 \times 10^{-12}$ ml molecule^{-1} s^{-1} at $1200 < T < 1700$ K . This value is adopted. It is consistent with the lower limit of about 2×10^{-12} ml molecule^{-1} s^{-1} given by Volpi and Zocchi[139] for $T \approx 310$ K .

Q20 Michael and Weston[140] suggest $k_{Q20} = 6 \times 10^{-13}$ ml molecule^{-1} s^{-1} at room temperature. Browne, Porter, Verlin and Clarke[141] interpret their work on the computer fitting of concentration profiles in flames as indicating the

quite inconsistent value of $k_{Q20} = 3 \times 10^{-10}$ exp(-9500/T) ml molecule^{-1} s^{-1}, but the uncertainties inherent in such a matching process are large. We list $k_{Q20} = 5 \times 10^{-10}$ exp(-2000/T) ml molecule^{-1} s^{-1}; the possible error bounds are wide indeed.

Q21 We are aware of no experimental work on this reaction. The pre-exponential factor in k_{Q21} is set equal to that in the rate coefficient of the formally similar reaction P4. The activation energy is obtained via arbitrary addition of 12 kJ mole^{-1} to the endothermicity.

Q22 Measurements of k_{Q22} at room temperature (e.g. Refs 142, 143, 137) result in a median value of about 7×10^{-13} ml molecule^{-1} s^{-1}. The activation energy is small[142] ($\approx$ 4 kJ mole^{-1}). With $k_{Q22} = 4 \times 10^{-12}$ exp(-500/T) ml molecule^{-1} s^{-1} and an equilibrium constant of 1.1×10^{-24} exp(+17000/T) ml molecule^{-1}, a value of 4×10^{12} exp(-17500/T) s^{-1} for k_{-Q22} results. This agrees adequately with the rather scattered measurements of k_{-Q22} at 600-800 K summarized by Benson and O'Neal[132].

Q23 Benson and Haugen[138,144] give $k_{-Q23} = 1.2 \times 10^{-9}$ exp(-15600/T) ml molecule^{-1} s^{-1} for conditions in which M is probably Ar. This corresponds to $k_{Q23} = 3.4 \times 10^{-34}$ exp(4800/T) ml^2 molecule^{-2} s^{-1}. For a typical flame molecule, this may reasonably be converted to the listed value of k_{Q23}, the uncertainty bounds in which are large.

Q24 It appears that no experimental work has been done on this reaction. The listed value is estimated by comparison with other three-body recombination rate coefficients, including k_{P1} and k_{A4}.

Q25 Baulch, Drysdale, Duxbury and Grant[3] decline to make a recommendation for k_{Q25} because of the paucity of experimental data. Peeters and Mahnen[119] suggest $k_{Q25} = 5 \times 10^{-11}$ ml molecule^{-1} s^{-1} at $1400 < T < 1800$ K. The activation energy is probably small[3]. The listed value is consistent with both suggestions and with the estimate of Demerjian, Kerr and Calvert[145] that $k_{Q25} \approx 1.7 \times 10^{-13}$ ml molecule^{-1} s^{-1} at about 300 K.

Q26 Westenberg and de Haas[146] tentatively suggest this reaction as a possible step in methane oxidation, with no associated rate coefficient given but in conjunction with the view that the reaction is fast by comparison with Q6. The listed rate coefficient is consistent with this view. It is estimated by comparison with other group Q rate coefficients, and in the light of the mechanistic as well as the kinetic uncertainties involved carries wide error bounds. The advantage of including this reaction in

calculations is that it affords, in combination with other reactions from groups Q and T, a formally complete interim description of the production of ions from a hydrocarbon in a flame. Such a description remains to be tested against results of the many experimental studies of hydrocarbon flame ionization, however.

R1 In the absence of any available experimental data for this reaction, the listed value of k_{R1} is estimated by comparison with those of rate coefficients for termolecular reactions on which measurements have been made.

R2 No experimental data are available for this reaction. The listed value is estimated by comparison with measured values for rate coefficients of formally similar bimolecular reactions.

R3 This rate coefficient is estimated in a manner similar to that in which k_{R2} was obtained.

R4 This rate coefficient is estimated in a manner similar to that in which k_{R2} was obtained.

S1 This rate coefficient was measured by Hayhurst and Kittelson[88]. The implied pre-exponential factor in k_{-S1} is higher than that suggested in Ref. 147, but the absolute value of k_{-S1} remains roughly the same as a result of a change in the formulation of the equilibrium constant K_{S1}.

S2 Cotton and Jenkins[148] have measured k_{S2} at 1570 K and 1800 K, finding $k_{S2} = 4.5 \times 10^{-12}$ ml molecule^{-1} s^{-1} at both temperatures. The listed value of k_{S2} gives 3.8×10^{-12} ml molecule^{-1} s^{-1} at 1570 K and 5.2×10^{-12} ml molecule^{-1} s^{-1} at 1800 K. It corresponds to $k_{-S2} = 1.5 \times 10^{-10}$ exp(-500/T) ml molecule^{-1} s^{-1}, with a small activation energy rather than the value decreasing with increasing temperature implied by the results of Ref. 148 used directly. Reaction S2, together with the other group S reactions influencing radical concentrations in flames, is worthy of further study.

S3 The formally similar reactions $LiOH + H \rightarrow Li + H_2O$, $NaOH + H \rightarrow Na + H_2O$, $KOH + H \rightarrow K + H_2O$ and $CsOH + H \rightarrow Cs + H_2O$ have been assigned values of 4.3×10^{-12} exp(-950/T), 3.5×10^{-12} exp(-1100/T), 3.6×10^{-12} exp(-1000/T) and 4.5×10^{-12} exp(-700/T) ml molecule^{-1} s^{-1} respectively (see the notes on reactions D4-D6 and D12 and the equilibrium constants for these reactions). The listed value of k_{S3} is similarly estimated.

S4 This rate coefficient is estimated by comparison with k_{D2} and k_{D3}.

S5 The equilibrium constant for this reaction is approximately given by $K_{S5} = 0.8 \exp(-4440/T)$. The activation energy in the listed value for k_{S5} is therefore sufficient to give the backward step of reaction S5 an activation energy of about 5 kJ $mole^{-1}$, which appears reasonable. The pre-exponential factor in k_{S5} is estimated by comparison with that in k_{-D3}; the collision cross section in k_{S5} might be expected to be somewhat larger, but the probability factor somewhat smaller, than the corresponding quantities in k_{-D3}.

S6 The listed rate coefficient is estimated by comparison with those for the reverse steps of group D reactions and with k_{V4}.

S7 Cotton and Jenkins[148] interpret their measurements of catalysed radical recombination rates in flames as indicating a value for k_{S7} at 1570-1800 K of about 3×10^{-12} ml $molecule^{-1}$ s^{-1}. This interpretation, however, is not based upon the best current value for the equilibrium constant of reaction S2, on which the value obtained for k_{S7} depends. Use of $K_{S2} = 0.27 \exp(-3180/T)$, in direct combination with the other data of Cotton and Jenkins[148], leads to $k_{S7} \approx 6 \times 10^{-10}$ ml $molecule^{-1}$ s^{-1}. This rate coefficient seems rather large for a bimolecular recombination reaction, but is nevertheless listed as the best at present available for use in flame calculations. Further work on this reaction is needed.

S8 This rate coefficient, like k_{S1}, is taken from the work of Hayhurst and Kittelson[88]. No positive identification of the products of dissociative recombination of $CaOH^+$ with e^- has yet been made.

S9 On the basis of comparison with other ion-molecule reaction rate coefficients (e.g. Ref. 75), one might expect k_{S9} to be at least $1 \times 10^{-10} \exp(-1000/T)$ ml $molecule^{-1}$ s^{-1}. Combined with $K_{S9} = 0.024 \exp(7100/T)$, this gives a value for k_{-S9} of $4 \times 10^{-9} \exp(-8100/T)$ ml $molecule^{-1}$ s^{-1}, which appears reasonable. The listed value of k_{S9} should not be in error by more than a factor of 30.

S21 This rate coefficient is estimated in a manner similar to that in which k_{-D6}, k_{-D5} and k_{-D4} were obtained.

S22 This rate coefficient is based on the work of Cotton and Jenkins[148], re-interpreted in the light of more recent values for the enthalpies and entropies of formation of BaO and BaOH [149]. See also the notes on reactions S2 and S7.

S23 This rate coefficient is taken from the work of Cotton and Jenkins[148].

S24 This rate coefficient is estimated by comparison with k_{V4} and other formally similar reactions.

S25 Jensen[147] estimates a value $\approx 10^{-7}$ ml molecule^{-1} s^{-1} for k_{S25} at 2000-2500 K. Similar values are obtained for the rate coefficients of dissociative recombination between $CaOH^+$ and e^- and between $SrOH^+ + e^-$ by Hayhurst and Kittelson[88]. The products of the reaction between $BaOH^+$ and e^- have not been identified, and may be Ba + OH or BaO + H . See also the notes on reaction S1.

S26 Jensen[147] estimates a value of about 10^{-7} ml molecule^{-1} s^{-1} for k_{S26} at 2000-2500 K. Similar values are obtained for the rate coefficients of dissociative recombination between $CaOH^+$ and e^- and between $SrOH^+$ and e^- by Hayhurst and Kittelson[88]. The products of the reaction between $BaOH^+$ and e^- have not been identified, and may be Ba + OH or BaO + H . See also the notes on reaction S1.

S27 This rate coefficient is estimated in a manner similar to that in which k_{S9} was obtained.

T3 The several rough estimates of this rate coefficient at flame temperatures $\approx$ 2000 K include 3×10^{-12} ml molecule^{-1} s^{-1} (Ref. 150), 5×10^{-12} ml molecule^{-1} s^{-1} (Ref. 151) and 3×10^{-13} ml molecule^{-1} s^{-1} (Ref. 152). The equilibrium constant of the reaction is approximately 1.2×10^{-5} exp(-1700/T) , so that a value for k_{T3} of 1×10^{-12} at 2000 K corresponds to $k_{-T3} = 2 \times 10^{-7}$ ml molecule^{-1} s^{-1} . Such a value for a dissociative recombination rate coefficient appears reasonable by comparison with, for example, k_{S1} , k_{S26} and k_{T11} . We suggest $k_{-T3} = 4 \times 10^{-4}\ T^{-1}$ ml molecule^{-1} s^{-1} , and hence $k_{T3} = 5 \times 10^{-9}\ T^{-1}$ exp(-1700/T) ml molecule^{-1} s^{-1} .

T4 Calcote and Jensen[70] use results from several sources in estimating $k_{T4} \approx 1 \times 10^{-8}$ ml molecule^{-1} s^{-1} at about 2000 K. Peeters and Van Tiggelen[151] find $k_{T4} = 7 \times 10^{-9}$ ml molecule^{-1} s^{-1} at similar temperatures. Both values are in reasonable agreement with theoretical estimates for this type of positive ion-molecule reaction (cf. Ref. 153), and the listed value should be reasonably realistic for the temperature range of interest.

T5 This rate coefficient is based upon the experimental work of Hayhurst and Telford[154,155].

T6 This rate coefficient is based upon the experimental work of Hayhurst and Telford[154,155].

T7 This rate coefficient is based upon the experimental work of Hayhurst and Telford[154,155].

T8 This rate coefficient is estimated by comparison with k_{T5}, k_{T6} and k_{T7}.

T9 The value listed for k_{T9} is based upon the work of Burdett, Hayhurst and Morley[89], who find $k_{T9}/k_{T11} = 0.11$ at 1800-2600 K. The products of this dissociative recombination were not identified by these authors and are in some doubt.

T10 The preliminary value listed for this rate coefficient is based upon unpublished work of Calcote and Kurzius[156].

T11 Several experimental determinations of the rate coefficient of dissociative recombination between H_3O^+ and e^- have been reported (e.g. Refs 82-87). The temperature dependence of the rate coefficient is not reliably established, but a T^{-1} dependence seems likely to be roughly correct. The experimental measurements then fit the expression $k_{T11} = 6 \times 10^{-4}\ T^{-1}$ ml molecule^{-1} s^{-1} reasonably well. This expression gives $k_{T11} = 3 \times 10^{-7}$ ml molecule^{-1} s^{-1} at 2000 K. Hayhurst and Telford[82] find a value for k_{-T11} of $6 \times 10^{-36} \exp(-14000/T)$ ml^2 molecule^{-2} s^{-1} at 2000-2450 K. With the equilibrium constant K_{T11} given by $6.5 \times 10^{28} \exp(14900/T)$ molecule ml^{-1}, this translates into $k_{T11} = 4 \times 10^{-7} \exp(900/T)$ ml molecule^{-1} s^{-1}, or 6×10^{-7} ml molecule^{-1} s^{-1} at 2000 K. The agreement with the direct measurements of k_{T11} is good, in the light of the various sources of possible experimental error, and supports the contention that the products of dissociative recombination are indeed H + H + OH. The recommended value of $6 \times 10^{-4}\ T^{-1}$ ml molecule^{-1} s^{-1} should be accurate to within a factor of 5 for typical flame conditions.

U1 The listed value is that given by Baulch, Drysdale, Horne and Lloyd[5].

U2 The listed value is that given by Baulch, Drysdale, Horne and Lloyd[5].

U3 Baulch, Drysdale, Horne and Lloyd[5] give $k_{U3} = 1.5 \times 10^{-32} \exp(300/T)$ ml^2 molecule^{-2} s^{-1} for $M \equiv H_2$ in the temperature range $230 < T < 700$ K, suggesting error bounds of ±50 per cent for this range. We retain this expression, which agrees nicely with the recent results of Oka, Singleton and

Cvetanovic[158], for flame third bodies, although the uncertainty factor must now be substantially greater.

U4 Baulch, Drysdale, Horne and Lloyd[5] suggest $k_{U4} = 8 \times 10^{-12}$ ml molecule^{-1} s^{-1} at 2000 K. Bulewicz and Sugden[159] find k_{U4} to be approximately 1×10^{-11} ml molecule^{-1} s^{-1} at temperatures between 1600 and 2000 K. Koshi, Ando, Oya and Asaba[160] give a value for k_{-U4} of 6.7×10^{-11} exp(-29000/T) ml molecule^{-1} s^{-1}, which may be translated into $k_{U4} = 9 \times 10^{-11}$ exp(-1100/T) ml molecule^{-1} s^{-1}. A temperature-independent value for k_{U4} of 8×10^{-12} ml molecule^{-1} s^{-1} should be accurate to within a factor of 10 for the temperature range of major interest in a flame context.

U5 Baulch, Drysdale, Horne and Lloyd[5] lean heavily on the work of Halstead and Jenkins[161] in recommending a value for k_{U5} of 6×10^{-11} ml molecule^{-1} s^{-1} at 2000 K. Within the limits of experimental error, this agrees with the work of Bulewicz and Sugden[159]. The listed value should be accurate to within a factor of 5 at flame temperatures.

U6 The listed value is that recommended in Ref. 5.

U7 The listed value is that recommended in Ref. 5.

V1 This estimate is taken from Ref. 162. See also the note to reaction V2.

V2 The listed value is taken from Ref. 162. Reactions V1-V4 are intended to account for catalysis of radical recombination in $H_2 + O_2 + N_2$ flames by iron, and the probable errors involved in using the set of rate coefficients and equilibrium constants given in Ref. 162 for calculations on other flames would be substantially smaller than the individual rate coefficient uncertainties suggest.

V3 The listed value is taken from Ref. 162. See also the note to reaction V2.

V4 The listed value is taken from Ref. 162. See also the note to reaction V2.

V11 The listed value is taken from Ref. 163. Reactions V11-V13 and V21-V23 are intended to account for catalysis of radical recombination in $H_2 + O_2 + N_2$ flames by molybdenum and tungsten respectively. The probable errors involved in using either set of rate coefficients and equilibrium constants for calculations on other flames would be substantially smaller than the individual rate coefficient uncertainties suggest.

V12 The listed value is taken from Ref. 163. See also the note to reaction V11.

V13 The listed value is taken from Ref. 163. See also the note to reaction V11.

V21 The listed value is taken from Ref. 163. See also the note to reaction V11.

V22 The listed value is taken from Ref. 163. See also the note to reaction V11.

V23 The listed value is taken from Ref. 163. See also the note to reaction V11.

V31 The listed value is an estimate taken from Ref. 164. See also the note on reaction V32.

V32 The listed value is taken from Ref. 164. Reactions V31-V34 are intended to account for catalysis of radical recombination in $H_2 + O_2 + N_2$ flames by cobalt, and the probable errors involved in using the set of rate coefficients and equilibrium constants given in Ref. 164 for calculations on other flames would be substantially smaller than the individual rate coefficient uncertainties suggest.

V33 The listed value is taken from Ref. 164. See also the note on reaction V32.

V34 The listed value is taken from Ref. 164. See also the note on reaction V32.

V41 This artificial overall rate coefficient is suggested by Jensen and Webb[165] as a means of describing the catalysis of radical recombination in flames by chromium observed by Bulewicz and Padley[166,167]. When it is used, the concentration of chromium is set equal to the total concentration of this metal in the flame, irrespective of what chromium compounds are formed therein.

V42 This artificial overall rate coefficient is suggested on the basis of the work of Bulewicz and Padley[166,168] and Jensen and Jones[163] as a means of describing the catalysis of radical recombination in flames by tin. When it is used, the concentration of tin oxide is set equal to the total concentration of tin in the flame, irrespective of what other tin-containing species may be present.

4 EQUILIBRIUM CONSTANTS AS FUNCTIONS OF TEMPERATURE

Reaction	Number	Equilibrium Constant	Source Reference
$O + O + M \rightarrow O_2 + M$	A1	7.1×10^{-26} exp(59580/T)	36
$O + H + M \rightarrow OH + M$	A2	8.8×10^{-25} exp(51610/T)	36
$H + H + M \rightarrow H_2 + M$	A3	3.8×10^{-25} exp(52650/T)	36
$H + OH + M \rightarrow H_2O + M$	A4	8.9×10^{-26} exp(60180/T)	36
$CO + O + M \rightarrow CO_2 + M$	A5	8.5×10^{-27} exp(62470/T)	36
$OH + H_2 \rightarrow H_2O + H$	B1	0.23 exp(7530/T)	36
$O + H_2 \rightarrow OH + H$	B2	2.26 exp(-1040/T)	36
$H + O_2 \rightarrow OH + O$	B3	12.4 exp(-7970/T)	36
$CO + OH \rightarrow CO_2 + H$	B4	9.6×10^{-3} exp(10860/T)	36
$OH + OH \rightarrow H_2O + O$	B5	0.102 exp(8570/T)	36
$CO + O_2 \rightarrow CO_2 + O$	B6	0.12 exp(2890/T)	36
$H + Cl_2 \rightarrow HCl + Cl$	C1	2.26 exp(23510/T)	36
$Cl + H_2 \rightarrow HCl + H$	C2	1.73 exp(-530/T)	36
$H_2O + Cl \rightarrow HCl + OH$	C3	7.4 exp(-8050/T)	36
$OH + Cl \rightarrow HCl + O$	C4	0.75 exp(510/T)	36
$H + HF \rightarrow H_2 + F$	C5	1.37 exp(-16200/T)	36
$H + F_2 \rightarrow HF + F$	C6	2.1 exp(50530/T)	36
$Li + HCl \rightarrow LiCl + H$	D1	4.2 exp(4610/T)	36
$Na + HCl \rightarrow NaCl + H$	D2	6.6 exp(-3610/T)	36
$K + HCl \rightarrow KCl + H$	D3	9.5 exp(-1960/T)	36
$Li + H_2O \rightarrow LiOH + H$	D4	13.9 exp(-10050/T)	36
$Na + N_2O \rightarrow NaOH + H$	D5	23 exp(-20900/T)	36
$K + H_2O \rightarrow KOH + H$	D6	28 exp(-19000/T)	36
$K + HBO_2 \rightarrow KBO_2 + H$	D7	60 exp(-3700/T)	36
$K + H_2WO_4 \rightarrow KHWO_4 + H$	D8	4.0 exp(2900/T)	36, 37
$K + H_2MoO_4 \rightarrow KHMoO_4 + H$	D9	3.6 exp(3500/T)	36, 38
$Na + HBO_2 \rightarrow NaBO_2 + H$	D10	37 exp(-4500/T)	36
$Li + HBO_2 \rightarrow LiBO_2 + H$	D11	46 exp(1680/T)	36
$Cs + H_2O \rightarrow CsOH + H$	D12	44 exp(-17300/T)	36
$H + Cl + M \rightarrow HCl + M$	E1	6.4×10^{-25} exp(52120/T)	36
$Cl + Cl + M \rightarrow Cl_2 + M$	E2	3.0×10^{-25} exp(28610/T)	36
$H + F + M \rightarrow HF + M$	E3	2.8×10^{-25} exp(68680/T)	36
$F + F + M \rightarrow F_2 + M$	E4	1.30×10^{-25} exp(18320/T)	36

Units of molecule ml^{-1} for concentrations used throughout.

Reaction	Number	Equilibrium Constant	Source Reference
$Li + OH + M \rightarrow LiOH + M$	F1	1.20×10^{-24} exp(50130/T)	36
$Na + OH + M \rightarrow NaOH + M$	F2	2.0×10^{-24} exp(39300/T)	36
$K + OH + M \rightarrow KOH + M$	F3	2.5×10^{-24} exp(41200/T)	36
$Li + Cl + M \rightarrow LiCl + M$	F4	2.7×10^{-24} exp(56740/T)	36
$Na + Cl + M \rightarrow NaCl + M$	F5	4.4×10^{-24} exp(48510/T)	36
$K + Cl + M \rightarrow KCl + M$	F6	6.3×10^{-24} exp(50170/T)	36
$Li^+ + e^- + M \rightarrow Li + M$	G1	1.18×10^{-21} exp(65350/T)	36
$Na^+ + e^- + M \rightarrow Na + M$	G2	1.18×10^{-21} exp(62410/T)	36
$K^+ + e^- + M \rightarrow K + M$	G3	1.18×10^{-21} exp(53130/T)	36
$Cs^+ + e^- + M \rightarrow Cs + M$	G4	1.18×10^{-21} exp(47200/T)	36
$In^+ + e^- + M \rightarrow In + M$	G5	1.18×10^{-21} exp(69900/T)	36, 169
$Li^+ + Cl^- \rightarrow Li + Cl$	H1	11.3 exp(20420/T)	36
$Na^+ + Cl^- \rightarrow Na + Cl$	H2	11.3 exp(17480/T)	36
$K^+ + Cl^- \rightarrow K + Cl$	H3	11.4 exp(8200/T)	36
$Li^+ + OH^- \rightarrow Li + OH$	H4	7.9 exp(41280/T)	36
$Na^+ + OH^- \rightarrow Na + OH$	H5	7.9 exp(38340/T)	36
$K^+ + OH^- \rightarrow K + OH$	H6	7.9 exp(29060/T)	36
$Li^+ + Cl^- + M \rightarrow LiCl + M$	H7	3.0×10^{-23} exp(77200/T)	36
$Na^+ + Cl^- + M \rightarrow NaCl + M$	H8	5.0×10^{-23} exp(66000/T)	36
$K^+ + Cl^- + M \rightarrow KCl + M$	H9	7.1×10^{-23} exp(58400/T)	36
$OH + e^- + M \rightarrow OH^- + M$	J1	1.5×10^{-22} exp(24030/T)	36
$Cl + e^- + M \rightarrow Cl^- + M$	J2	1.1×10^{-22} exp(44860/T)	36
$HCl + e^- \rightarrow Cl^- + H$	J3	195 exp(-7600/T)	36
$HBO_2 + e^- \rightarrow BO_2^- + H$	J4	660 exp(-8160/T)	36
$H_2MoO_4 + e^- \rightarrow HMoO_4^- + H$	J5	24 exp(500/T)	38
$H_2WO_4 + e^- \rightarrow HWO_4^- + H$	J6	25 exp(1300/T)	37
$H_2O + e^- \rightarrow OH^- + H$	J7	1600 exp(-36060/T)	36
$HMoO_4^- + H \rightarrow MoO_3^- + H_2O$	J8	0.85 exp(10400/T)	38
$HWO_4^- + H \rightarrow WO_3^- + H_2O$	J9	0.87 exp(5700/T)	37
$O_2 + e^- + M \rightarrow O_2^- + M$	J10	1.3×10^{-21} exp(7400/T)	36
$LiH_2O^+ + M \rightarrow Li^+ + H_2O + M$	L1	2.2×10^{23} exp(-23000/T)	78, 81
$NaH_2O^+ + M \rightarrow Na^+ + H_2O + M$	L2	1.0×10^{23} exp(-15000/T)	78, 79, 81
$KH_2O^+ + M \rightarrow K^+ + H_2O + M$	L3	3.6×10^{22} exp(-10000/T)	78, 79, 81
$LiH_2O^+ + e^- \rightarrow Li + H_2O$	L4	260 exp(42350/T)	36, 78, 81
$NaH_2O^+ + e^- \rightarrow Na + H_2O$	L5	120 exp(47410/T)	36, 78, 79, 81
$KH_2O^+ + e^- \rightarrow K + H_2O$	L6	43 exp(43130/T)	36, 78, 79, 81
$LiH_2O^+ + Cl^- \rightarrow Li + Cl + H_2O$	L7	2.5×10^{24} exp(-2510/T)	36, 78, 81

Units of molecule ml^{-1} for concentrations used throughout.

Reaction	Number	Equilibrium Constant	Source Reference
$NaH_2O^+ + Cl^- \rightarrow Na + Cl + H_2O$	L8	1.1×10^{24} exp(2550/T)	36, 78, 79, 81
$KH_2O^+ + Cl^- \rightarrow K + Cl + H_2O$	L9	4.0×10^{23} exp(-1730/T)	36, 78, 79, 81
$LiH_2O^+ + OH^- \rightarrow Li + OH + H_2O$	L10	1.7×10^{24} exp(18310/T)	36, 78, 81
$NaH_2O^+ + OH^- \rightarrow Na + OH + H_2O$	L11	7.9×10^{23} exp(23380/T)	36, 78, 79, 81
$KH_2O^+ + OH^- \rightarrow K + OH + H_2O$	L12	2.8×10^{23} exp(19100/T)	36, 78, 79, 81
$O + Cl + M \rightarrow ClO + M$	M1	9.5×10^{-25} exp(31400/T)	36
$Li + ClO \rightarrow LiCl + O$	M2	3.6 exp(24930/T)	36
$Na + ClO \rightarrow NaCl + O$	M3	5.7 exp(16700/T)	36
$K + ClO \rightarrow KCl + O$	M4	8.3 exp(18360/T)	36
$H + ClO \rightarrow HCl + O$	M5	0.87 exp(20320/T)	36
$O + ClO \rightarrow O_2 + Cl$	M6	9.4×10^{-2} exp(27780/T)	36
$OH + ClO \rightarrow HO_2 + Cl$	M7	0.125 exp(-376/T)	36
$Na + O_2 + M \rightarrow NaO_2 + M$	N2	1.36×10^{-24} exp(30950/T)	97
$K + O_2 + M \rightarrow KO_2 + M$	N3	1.5×10^{-24} exp(32700/T)	97
$NaO_2 + Cl \rightarrow NaCl + O_2$	N5	3.2 exp(17560/T)	36, 97
$KO_2 + Cl \rightarrow KCl + O_2$	N6	4.2 exp(17500/T)	36, 97
$NaO_2 + H_2 \rightarrow NaOH + OH$	N8	42 exp(-680/T)	36, 97
$KO_2 + H_2 \rightarrow KOH + OH$	N9	46 exp(-520/T)	36, 97
$NaO_2 + OH \rightarrow NaOH + O_2$	N11	1.5 exp(8300/T)	36, 97
$KO_2 + OH \rightarrow KOH + O_2$	N12	1.7 exp(8500/T)	36, 97
$Na(^2S_{1/2}) + H + OH \rightarrow Na(^2P_{1/2}) + H_2O$	N13	8.9×10^{-26} exp(35770/T)	36
$Na(^2S_{1/2}) + H + OH \rightarrow Na(^2P_{3/2}) + H_2O$	N14	1.78×10^{-25} exp(35750/T)	36
$Na(^2S_{1/2}) + H + H \rightarrow Na(^2P_{1/2}) + H_2$	N15	3.8×10^{-25} exp(28240/T)	36
$Na(^2S_{1/2}) + H + H \rightarrow Na(^2P_{3/2}) + H_2$	N16	7.6×10^{-25} exp(28220/T)	36
$Na(^2S_{1/2}) + O + O \rightarrow Na(^2P_{1/2}) + O_2$	N17	7.1×10^{-26} exp(35170/T)	36
$Na(^2S_{1/2}) + O + O \rightarrow Na(^2P_{3/2}) + O_2$	N18	1.42×10^{-25} exp(35150/T)	36
$Na(^2S_{1/2}) + M \rightarrow Na(^2P_{1/2}) + M$	N19	1.00 exp(-24410/T)	36
$Na(^2S_{1/2}) + M \rightarrow Na(^2P_{3/2}) + M$	N20	2.00 exp(-24430/T)	36
$Na(^2P_{1/2}) + M \rightarrow Na(^2P_{3/2}) + M$	N24	2.00 exp(-25/T)	36
$K(^2S_{1/2}) + H + OH \rightarrow K(^2P_{1/2}) + H_2O$	N25	8.9×10^{-26} exp(41490/T)	36
$K(^2S_{1/2}) + H + OH \rightarrow K(^2P_{3/2}) + H_2O$	N26	1.78×10^{-25} exp(41410/T)	36
$K(^2S_{1/2}) + H + H \rightarrow K(^2P_{1/2}) + H_2$	N27	3.8×10^{-25} exp(33960/T)	36
$K(^2S_{1/2}) + H + H \rightarrow K(^2P_{3/2}) + H_2$	N28	7.6×10^{-25} exp(33880/T)	36
$K(^2S_{1/2}) + O + O \rightarrow K(^2P_{1/2}) + O_2$	N29	7.1×10^{-26} exp(40890/T)	36
$K(^2S_{1/2}) + O + O \rightarrow K(^2P_{3/2}) + O_2$	N30	1.42×10^{-25} exp(40810/T)	36

Units of molecule ml^{-1} for concentrations used throughout.

Reaction	Number	Equilibrium Constant	Source Reference
$K(^2S_{1/2}) + M \rightarrow K(^2P_{1/2}) + M$	N31	1.00 exp(-18690/T)	36
$K(^2S_{1/2}) + M \rightarrow K(^2P_{3/2}) + M$	N32	2.00 exp(-18770/T)	36
$K(^2P_{1/2}) + M \rightarrow K(^2P_{3/2}) + M$	N35	2.00 exp(-83/T)	36
$Na + HO_2 \rightarrow NaO_2 + H$	N38	1.20 exp(7490/T)	36, 97
$K + HO_2 \rightarrow KO_2 + H$	N41	1.35 exp(9230/T)	36, 97
$H + O_2 + M \rightarrow HO_2 + M$	P1	1.18×10^{-24} exp(23460/T)	36
$Cl + HO_2 \rightarrow HCl + O_2$	P2	0.56 exp(28670/T)	36
$H + HO_2 \rightarrow OH + OH$	P3	9.3 exp(20180/T)	36
$H + HO_2 \rightarrow H_2 + O_2$	P4	0.33 exp(29200/T)	36
$H_2 + HO_2 \rightarrow H_2O + OH$	P5	2.2 exp(27710/T)	36
$CO + HO_2 \rightarrow CO_2 + OH$	P6	0.090 exp(31050/T)	36
$O + HO_2 \rightarrow O_2 + OH$	P7	0.75 exp(28160/T)	36
$OH + HO_2 \rightarrow H_2O + O_2$	P8	0.076 exp(36730/T)	36
$CHO + O \rightarrow CO + OH$	Q1	0.34 exp(44400/T)	36
$CHO + OH \rightarrow CO + H_2O$	Q2	0.034 exp(53070/T)	36
$CO + H + M \rightarrow CHO + M$	Q3	2.7×10^{-24} exp(7100/T)	36
$CHO + H \rightarrow CO + H_2$	Q4	0.145 exp(45520/T)	36
$CH_4 + H \rightarrow CH_3 + H_2$	Q5	23	36
$CH_4 + O \rightarrow CH_3 + OH$	Q6	58 exp(-1100/T)	36
$CH_4 + OH \rightarrow CH_3 + H_2O$	Q7	5.8 exp(7530/T)	36
$CH_2O + OH \rightarrow CHO + H_2O$	Q8	2.8 exp(15160/T)	36
$CH_2O + H \rightarrow CHO + H_2$	Q9	11.9 exp(7610/T)	36
$CH_2O + O \rightarrow CHO + OH$	Q10	27 exp(6530/T)	36
$CH_3 + OH \rightarrow CH_2O + H_2$	Q11	0.034 exp(36040/T)	36
$CH_3 + O_2 \rightarrow CH_2O + OH$	Q12	0.95 exp(26970/T)	36
$CH_3 + O \rightarrow CH_2O + H$	Q13	0.078 exp(34960/T)	36
$CH_3 + H + M \rightarrow CH_4 + M$	Q14	4×10^{-27} exp(54600/T)	36
$CH_3 + CH_3 \rightarrow C_2H_6$	Q15	8.8×10^{-28} exp(43880/T)	36, 170-173
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	Q16	21.7 exp(1140/T)	36, 170-173
$C_2H_5 + H \rightarrow C_2H_4 + H_2$	Q17	0.35 exp(35700/T)	36, 170-173
$C_2H_4 + H \rightarrow C_2H_3 + H_2$	Q18	6.3 exp(-590/T)	36, 170-173
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	Q19	1.35 exp(32300/T)	36, 170-173
$C_2H_2 + H \rightarrow C_2H + H_2$	Q20	4.5 exp(-2600/T)	36
$C_2H + H \rightarrow C_2 + H_2$	Q21	2.3 exp(-16580/T)	36
$C_2H_4 + H \rightarrow C_2H_5$	Q22	1.1×10^{-24} exp(17000/T)	36, 170-173
$C_2H_2 + H + M \rightarrow C_2H_3 + M$	Q23	2.8×10^{-25} exp(20400/T)	36, 170-173
$C_2 + H + M \rightarrow C_2H + M$	Q24	1.65×10^{-25} exp(69200/T)	36
$CHO + O_2 \rightarrow CO + HO_2$	Q25	0.44 exp(16330/T)	36
$CH_3 + O \rightarrow CH + H_2O$	Q26	3.5 exp(5940/T)	36

Units of molecule ml^{-1} for concentrations used throughout.

Reaction	Number	Equilibrium Constant	Source Reference
$Cl + OH + M \rightarrow HOCl + M$	R1	1.9×10^{-25} exp(29600/T)	36
$HOCl + H \rightarrow ClO + H_2$	R2	1.8 exp(3250/T)	36
$HOCl + OH \rightarrow ClO + H_2O$	R3	0.41 exp(10780/T)	36
$HOCl + O \rightarrow ClO + OH$	R4	4.0 exp(2210/T)	36
$CaOH^+ + e^- \rightarrow Ca + OH$	S1	84 exp(20520/T)	36, 147, 174
$CaOH + H \rightarrow CaO + H_2$	S2	0.27 exp(-3180/T)	36, 149, 175, 176
$CaOH + H \rightarrow Ca + H_2O$	S3	0.018 exp(9320/T)	36, 149
$Ca + HCl \rightarrow CaCl + H$	S4	22.4 exp(-4200/T)	36
$CaCl_2 + H \rightarrow CaCl + HCl$	S5	0.80 exp(-4440/T)	36
$Ca(OH)_2 + H \rightarrow CaOH + H_2O$	S6	0.24 exp(-10600/T)	36, 148, 149, 177
$CaO + H_2O \rightarrow Ca(OH)_2$	S7	6.0×10^{-24} exp(45250/T)	36, 148, 149, 175-177
$CaOH^+ + e^- \rightarrow CaO + H$	S8	290 exp(15500/T)	36, 147, 149, 174-176
$CaOH^+ + H \rightarrow Ca^+ + H_2O$	S9	0.024 exp(7100/T)	36, 147, 174
$BaOH + H \rightarrow Ba + H_2O$	S21	0.0144 exp(4230/T)	149
$BaO + H_2O \rightarrow Ba(OH)_2$	S22	1.32×10^{-23} exp(30290/T)	148, 149, 36, 177
$BaOH + H \rightarrow BaO + H_2$	S23	0.12 exp(10840/T)	36, 149
$Ba(OH)_2 + H \rightarrow BaOH + H_2O$	S24	0.24 exp(11520/T)	36, 148, 149, 177
$BaOH^+ + e^- \rightarrow Ba + OH$	S25	66 exp(7400/T)	147
$BaOH^+ + e^- \rightarrow BaO + H$	S26	126 exp(21540/T)	36, 147
$BaOH^+ + H \rightarrow Ba^+ + H_2O$	S27	0.019 exp(4440/T)	36, 169, 147
$CH + O \rightarrow CHO^+ + e^-$	T3	1.24×10^{-5} exp(-1670/T)	36
$CHO^+ + H_2O \rightarrow H_3O^+ + CO$	T4	0.27 exp(15250/T)	36
$H_3O^+ + Li \rightarrow Li^+ + H_2O + H$	T5	4.9×10^{24} exp(9780/T)	36
$H_3O^+ + Na \rightarrow Na^+ + H_2O + H$	T6	4.9×10^{24} exp(12700/T)	36
$H_3O^+ + K \rightarrow K^+ + H_2O + H$	T7	4.9×10^{24} exp(22000/T)	36
$H_3O^+ + In \rightarrow In^+ + H_2O + H$	T8	4.9×10^{24} exp(5180/T)	36,169
$H_3O^+ + Cl^- \rightarrow H_2O + H + Cl$	T9	5.5×10^{25} exp(30200/T)	36
$H_3O^+ + OH^- \rightarrow H_2O + H + OH$	T10	4.0×10^{25} exp(51020/T)	36
$H_3O^+ + e^- \rightarrow H + H + OH$	T11	6.5×10^{28} exp(14900/T)	36
$NO + NO \rightarrow N_2O + O$	U1	0.026 exp(-19100/T)	36
$N_2O + H \rightarrow N_2 + OH$	U2	19 exp(33200/T)	36
$NO + H + M \rightarrow HNO + M$	U3	3.1×10^{-25} exp(24640/T)	36
$HNO + N \rightarrow NO + H_2$	U4	1.30 exp(27900/T)	36
$HNO + OH \rightarrow NO + H_2O$	U5	0.31 exp(35450/T)	36
$N_2 + O \rightarrow NO + N$	U6	4.6 exp(-37900/T)	36
$N + O_2 \rightarrow NO + O$	U7	4.7 exp(16120/T)	36

Units of molecule ml^{-1} for concentrations used throughout.

Reaction	Number	Equilibrium Constant	Source Reference
$Fe + H_2O \rightarrow FeOH + H$	V1	66 exp(-16100/T)	36, 162, 178
$FeOH + H \rightarrow FeO + H_2$	V2	0.044 exp(5400/T)	36, 162, 178
$FeO + H_2O \rightarrow Fe(OH)_2$	V3	9.0×10^{-25} exp(35500/T)	36, 162, 178
$Fe(OH)_2 + H \rightarrow FeOH + H_2O$	V4	10 exp(11700/T)	36, 162, 178
$HMoO_3 + H \rightarrow MoO_3 + H_2$	V11	0.037 exp(19600/T)	163
$MoO_3 + H_2O \rightarrow H_2MoO_4$	V12	4.3×10^{-23} exp(24700/T)	36
$H_2MoO_4 + H \rightarrow HMoO_3 + H_2O$	V13	0.23 exp(8350/T)	163
$HWO_3 + H \rightarrow WO_3 + H_2$	V21	0.037 exp(9000/T)	163
$WO_3 + H_2O \rightarrow H_2WO_4$	V22	1.4×10^{-23} exp(39500/T)	36
$H_2WO_4 + H \rightarrow HWO_3 + H_2O$	V23	0.73 exp(4150/T)	163
$Co + OH \rightarrow CoO + H$	V31	0.45 exp(1200/T)	164
$CoOH + H \rightarrow CoO + H_2O$	V32	0.25 exp(17700/T)	164
$CoO + H_2O \rightarrow Co(OH)_2$	V33	2.7×10^{-24} exp(24950/T)	164
$Co(OH)_2 + H \rightarrow CoOH + H_2O$	V34	0.56 exp(10000/T)	164
$H + H(+ Cr) \rightarrow H_2(+ Cr)$	V41	3.8×10^{-25} exp(52650/T)	36
$H + H(+ SnO) \rightarrow H_2(+ SnO)$	V42	3.8×10^{-25} exp(52650/T)	36

Units of molecule ml^{-1} for concentrations used throughout.

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178	Jensen, D.E. Jones, G.A.	Iron compounds in flames. Relative stabilities of Fe, FeO, FeOH and $Fe(OH)_2$. J. Chem. Soc. Faraday Trans. I 69, 1448 (1973)
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Abstract

A list of recommended rate coefficients for chemical reactions occurring in flames is given. Rate coefficients, expressed as functions of temperature for the range $1000 \leq T \leq 3000$ K, are either taken from experiments described in the scientific literature or estimated by comparison with rate coefficients for analogous reactions. Brief notes on the origins of recommended coefficients are included and rough uncertainties are attached to the listed values. A table showing reaction equilibrium constants as functions of temperature is also provided.

$1000 < \alpha = T < \alpha = 3000$ K