Evaluated chemical kinetic data for the reactions of atomic oxygen $O(^3P)$ with unsaturated hydrocarbons

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Chemical kinetic data for reactions of $O(^3P)$ atoms with unsaturated hydrocarbons are compiled and critically evaluated. Specifically, the reactions considered include the interactions of the ground electronic state of oxygen atoms, $O(^3P)$, with alkenes, cycloalkenes, halogen substituted alkenes and ketenes, alkynes, halogen substituted alkynes, aromatic hydrocarbons, halogen substituted aromatic hydrocarbons and pyridine. All kinetic data considered were restricted to gas phase reactions. "Recommended" values of the rate parameters have been assessed and conservative uncertainty limits assigned to them.

Key words: alkenes; alkynes; aromatic hydrocarbons; Arrhenius parameters; atomic oxygen; chemical kinetics; evaluated kinetic data; ketenes; $O(^3P)$; pyridine; rate of reaction; recommended kinetic parameters; unsaturated hydrocarbons.

Contents

1. Introduction

1.1. Overview

The present evaluation of chemical kinetic data for the elementary reactions of $O(^3P)$ atoms with unsaturated hydrocarbons is a part of a larger effort directed towards the development of a comprehensive general evaluated chemical kinetic data base. More specifically, it is a part of the broader data base for all $O(^3P)$ reactions, with both organic and inorganic reactants. It is thus also a part of an extensive data base, currently developed by the Chemical Kinetics Data Center of the National Bureau of Standards, dealing with the chemical oxidative processes, in particular those involved in thermal combustion and in the atmospheric chemistry. The data bases are intended to provide easily accessible sources of critically evaluated rate data for use in computer modeling and in general research needed for better understanding of these important and at times remarkably complex phenomena. In addition, in view of the fundamental importance of $O(^3P)$ reactions with the unsaturated hydrocarbons, a critically evaluated set of their rate constants may be expected to help establish more precisely the relationships between the rates of elementary reactions and the molecular structure of the reactants, possibly permitting extrapolations of rate data to reactants for which reliable information is not available. An example of such correlations is the electrophilic trend[1-3] in $O(^3P)$ reactions with alkenes. Well established kinetic behavior of $O(^3P)$ atoms may be expected also to serve as a model for other atom-unsaturated hydrocarbon reactions.

The main object of the evaluation has been to compile as many as possible of the published values of reaction rates of the elementary steps involved in the reactions of $O(^3P)$ atoms with the unsaturated hydrocarbons and to use them to arrive at an estimate of the "recommended" (or "preferred") values of the kinetic parameters and their uncertainties.

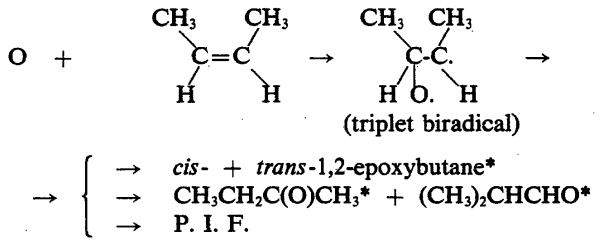
1.2. Reaction Mechanisms

Interaction of a ground state oxygen atom, $O(^3P)$, with an unsaturated hydrocarbon molecule may in principle lead to any of the following three types of chemical change: 1) "abstraction" by the O atom of a H atom from the hydrocarbon, 2) "addition" of the O atom to the hydrocarbon, and 3) "replacement" by the O atom of an atom or atomic group (radical) from the hydrocarbon. "Replacement" itself is of necessity initially an addition, combined with subsequent or simultaneous fragmentation of the initial adduct. (The term "displacement" is frequently used for a "replacement" reaction in which the initial addition and the departure of the displaced atom or radical are believed to take place simultaneously). "Insertion", the particular type of addition in which the atom inserts into CH bonds of hydrocarbons, is spin forbidden for $O(^3P)$ atoms and does not occur (although it is not spin forbidden for $O(^1D_2)$ atoms and occurs readily[4]).

It is not feasible to describe here in detail all aspects of the mechanisms of $O(^3P)$ reactions with unsaturated hydrocarbons. The mechanism of the reactions with alkenes, which provide a model for $O(^3P)$ reactions with other unsaturated hydrocarbons, will be briefly summarized in the following. The earlier reviews[2,5-7] discuss the reaction mechanisms in considerable detail and provide lists of original references. The more recent review by Cvetanović and Singleton[3] discusses also some more recent experimental and theoretical work related to the mechanisms of these reactions.

The pioneering research of the present author has shown that addition of $O(^3P)$ atoms to the CC double bond is the main and perhaps frequently the exclusive initial process in the reaction of simple olefins with $O(^3P)$ atoms. At least at not too elevated temperature and with $O(^3P)$ atoms not kinetically excited ("hot"), abstraction cannot compete effectively with the very rapid $O(^3P)$ addition to the double bond. However, at sufficiently high temperature, or with sufficiently "hot" $O(^3P)$ atoms, abstraction of H atoms should be expected to become more important.[3]

Two general types of final products due to the initial addition of $O(^3P)$ to alkenes are observed: 1) stabilized adducts and 2) the products formed by fragmentation of the initial adducts (including products formed in secondary reactions of the free radical fragments). The stabilized adducts are of two types: 1) the epoxides (formed by attachment of O atoms to the double bond) and 2) products formed by molecular rearrangement of the initial adducts, which are almost exclusively carbonyl compounds (aldehydes and ketones). The rearrangement products are formed by a 1,2 C to C shift of an H atom (or less frequently radical group) from the C atom to which $O(^3P)$ adds to the other C atom of the original double bond. Formation of epoxides is nonstereospecific: with either *cis*- or *trans*-2-butene, for example, both *cis*- and *trans*-2-butene oxide are produced and their ratio is different in the two reactions and is also temperature dependent. The overall process can be illustrated in a simplified manner using the $O(^3P)$ reaction with *cis*-2-butene as an example:



[P.I.F. = Pressure Independent Fragmentation (into CH_3, etc.)].

In order to explain the observed products, and taking into account the spin conservation rule, it is necessary to postulate that the initial adduct is a triplet biradical. This intermediate subsequently rapidly rearranges into highly vibrationally excited ("hot") epoxides and carbonyl compounds or undergoes a rapid "pressure independent" fragmentation (which may also include displacements, as defined earlier in this section). The "hot" epoxides and carbonyl compounds undergo at lower pressures a "pressure dependent fragmentation" and tend to be collisionally stabilized at higher pressures. As expected, the pressure dependent fragmentation is suppressed in condensed media[3,8].

The general mechanism of O atom addition to alkynes[7] is analogous to that for the addition to alkenes. Fewer mechanistic studies have been done for $O(^3P)$ additions to aromatic hydrocarbons. In the $O(^3P)$ reaction with benzene[9] the main product is a non-volatile material difficult to characterize. However, the direct adduct, phenol, is also formed in smaller amounts (about 13% of the benzene consumed). In the reaction with toluene[10], 15–20% of the O atoms reacted are recovered as the direct adduct, cresol (*o*-cresol and *p*-cresol, in a ratio of about 3:1, with very little or no *m*-cresol).

Reaction "branching ratios" are generally defined by assigning the total yields of different sets of the final products to the assumed simultaneously occurring distinct reaction channels. However, since in the reactions included in the present evaluation, $O(^3P)$ addition predominates and it forms a highly reactive and energy rich transient intermediate, the distribution of the final products is frequently strongly influenced by secondary reactions and by the particular experimental conditions employed in kinetic studies. In fact, not too many kinetic studies include comprehensive quantitative product determinations. Seemingly conflicting results are therefore not uncommon. On the other hand, within the range of experimental conditions explored so far, the overall rate constants at a fixed temperature seem to be unaffected by substantial variation in experimental conditions, although it is possible that they will exhibit some decrease

when the pressure is drastically lowered and the "single collision" conditions are approached. The present evaluation therefore deals primarily with the overall rate constants. Alternative reaction paths are indicated for a number of reactions but without attempting to make a comprehensive selection of preferred values of branching ratios.

1.3. Selection of Recommended Rate Parameters and their Uncertainty Factors

As a result of potential presence of unknown ("hidden") systematic errors in the measured values of rate constants of a reaction, most frequently obtained by different techniques and in different laboratories, there are no standard statistical methods for a quantitative evaluation of the expected "best" value and its confidence limits. When there is close agreement (within the combined imprecisions), of two or preferably more values obtained by different techniques, it is reasonable to assume that systematic errors are probably less important than the random errors. In such cases, use of standard weighted least squares techniques may be justified and is equivalent to treating any residual systematic errors as random errors.[11] In the present evaluation, the weighted least squares procedures were generally used to calculate the mean value and when an additive (±) error is given, it represents one standard deviation of the mean thus evaluated. Based on intuition and judgment of the evaluator, smaller (and, in one or two rare cases, zero) weights were assigned to some literature values. (For example, for the O atom reaction with propylene at 298 K, one listed value is two orders of magnitude smaller than the other values. It is therefore assigned zero weight while the statistical weights for the other values are unity or close to unity.)

Since the procedure used is of necessity subjective, conservatively estimated probable overall uncertainties were assigned to the selected "recommended" values of k and the Arrhenius A factor. It was found convenient to express these uncertainties in k and A in the form of uncertainty factors (which must not be taken to imply that the errors in the rate constants are necessarily log-normally distributed). The uncertainties assigned to the Arrhenius B, expressed as additive (±) deviations, are also approximate estimates.

The evaluation covers the investigated (and documented in the literature) $O(^3P)$ reactions with alkenes, cycloalkenes, halogen substituted alkenes, ketenes, alkynes, halogen substituted alkynes, aromatic hydrocarbons, halogen substituted aromatic hydrocarbons, and pyridine. Only gas phase reactions have been considered. For previous evaluations of kinetic data for some of these reaction systems, see, for example, Refs. 12, 3, and 13.

1.4. Organization

The material presented in this article is organized into five sections. Section 1 is the Introduction. Section 2 gives a brief summary of the adopted symbols and units. Section 3 contains a table of all recommended kinetic parameters and the page numbers indicating the locations of the detailed tabulations of the kinetic data for the listed reactions. Section 4 contains four tables of the chemical kinetic data for $O(^3P)$ reactions with 1) alkenes, 2) haloalkenes and ketenes, 3) alkynes, and 4) aromatic hydrocarbons, including pyridine. Section 5 contains the list of references for the tabulated recommended kinetic parameters and chemical kinetic data.

1.5. Guide to Summary of Recommended Rate Parameters

The Table in Sec. 3 summarizes the recommended values of the kinetic parameters for the listed gas phase second order reactions. The information is displayed in 7 columns. Column 1 ("Reaction") contains the reaction formula and the chemical name of the species reacting with $O(^3P)$ atoms. If Column 2 ("T/K") contains a single temperature, e.g. 298, the value in Column 3 ("k,A") is k at that temperature; if it contains a temperature range, e.g. 200–500, the value in Column 3 is the Arrhenius A. The units of k and A are $cm^3mol^{-1}s^{-1}$ and their values are given in exponential form, written as (1.00±0.10)(11), which signifies $(1.00\pm0.10)\times10^{11}$. For recommended values of k and A, the additive (±) errors, when given, represent one standard deviation of their weighted least squares evaluations.

Columns 4 ("n") and 5 ("B") contain, if applicable, the n and B parameters in extended Arrhenius Eq. $k=A(T/298)^n\exp(-B/T)$. Column 6 ("k err. factor") contains the assigned uncertainty factors of k and A, and Column 7 ("Page") lists the page number showing the location of detailed tabulation of kinetic data for the reaction.

1.6. Guide to Chemical Kinetic Data Tables

The formats of the four Chemical Kinetic Data Tables in this section are identical. All kinetic data listed are for gas phase reactions.

The data in the tables are divided into eight columns. Column 1 ("Reaction, Reference Code, Notes") contains: 1) Reaction Formula, 2) Chemical names of the two reactants and occasionally, in parentheses, a synonym of the hydrocarbon reacting with $O(^3P)$, 3) the Reference Code and 4) Notes relevant to the data entered. When, for brevity, the reference code is omitted from Column 1 of a data line, it is the same as the closest reference code in Column 1 in one of the preceding data lines. The Reference Code consists of the last two digits of the year of publication, followed by the first three letters of the names of the first and second author (if present) separated by a slash. An integer index is attached at the end when it is necessary to differentiate between otherwise identical Codes. This is illustrated by the Code 74 ATK/PIT2. Column 2 ("Data type") contains the two-character Data Type Codes listed in Sec. 2. If Column 3 ("T/K") contains a single temperature, e.g., 298, the value in Column 4 ("k,k/k(ref),A,A/A(ref)") is

k (or k/k(ref)) at that temperature; if it contains a temperature range, e.g. 200–500, the value in Column 4 is the Arrhenius A parameter (or A/A(ref)). Column 5 ("n") and Column 6 ("B,$B-B$(ref)"), respectively, contain, when applicable, the n and B (or $B-B$(ref)) parameters in the extended Arrhenius Eq. $k=A(T/298)^n\exp(-B/T)$. k(ref), A(ref) and B(ref) are the kinetic parameters of reference reaction in relative rate determinations. Column 7 ("k,A units") specifies the reaction order and thus defines the units of k and A, as listed in Sec. 2. Column 8 ("k err. factor") lists the overall uncertainty factors assigned to k and A.

1.7. Acknowledgments

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2. Summary of Symbols and Units

Reaction Phase Codes:
G = gas, L = liquid, S = solid, M = mixed phases (gas-liquid, gas-solid, liquid-solid, gas-liquid-solid)

Data Type Codes:
EX (experimentally measured absolute value),
RL (experimentally measured relative value),
RN (RL normalized to absolute value),
TH (theoretical value),
DE (derived indirectly, e.g., using reverse rate and equilibrium constant, or computer simulation of a complex mechanism)
CO (computed numerically),
ES (estimated, by analogy, etc.),
SE (selected in the literature as probable "best" value),
RE (currently recommended value).

Type of excitation:
(EXV) (vibrationally excited)
(EXT) (translationally excited)
(EXE) (electronically excited)
(EXEV) (electronically and vibrationally excited), etc.

Decadic exponent notation: 1.2(11) (stands for 1.2×10^{11})

Temperature (T): in kelvins (K).

Arrhenius parameters are defined by
$k=A(T/298)^n\exp(-B/T)$

Unit Codes for k, k/k(ref), A, A/A(ref):
1 (s^{-1}),
2 ($cm^3mol^{-1}s^{-1}$),
3 ($cm^6mol^{-2}s^{-1}$),
1/1, 2/2, etc. (dimensionless),
2/1 (cm^3mol^{-1}), etc.

($T/298$) and n (the exponent of T) are dimensionless.

Units for B, $B-B$(ref): kelvins (K). (Activation energy $E=R\times B$).

k(ref), A(ref) and B(ref) are the values for the "reference reaction" in relative rate determinations.

k err. factor: Estimated overall Uncertainty Factor. It multiplies and divides k or A to indicate approximate error limits. It does not imply that errors in k are necessarily lognormally distributed.

3. Index of Reactions and Summary of Recommended Rate Parameters

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + ALKENE REACTIONS:						
O + CH_2=CH_2 → products	298	(4.40±0.56)(11)			1.2	271
O + Ethene	200-500	6.4(12)	*)	800±200	1.5	
O + CH_2=CH_2 → CH_3 + ·CHO						274
O + Ethene						
O + CH_2=CH_2(EXV) → products						275
O + Ethene(EXV)						
O + CD_2=CD_2 → products	298	4.4(11)			1.2	275
O + Ethene-d_4	200-500	6.4(12)	*)	800±200	1.5	
O + CH_2=C=CH_2 → products	298	7.4(11)			1.2	276
O + 1,2-Propadiene	290-500	1.7(13)	*)	930±100	1.5	
O + CH_2=C=CH_2 → H + [C_3H_3O]·						276
O + 1,2-Propadiene						
O + CH_3CH=CH_2 → products	298	(2.4±0.3)(12)			1.2	276
O + 1-Propene	290-450	6.1(12)	*)	280±100	1.5	
O + CD_3CD=CD_2 → products	298	2.4(12)			1.2	278
O + 1-Propene-d_6						
O + CH_2=CHCH=CH_2 → products	298	(1.19±0.10)(13)			1.2	279
O + 1,3-Butadiene	290-500	1.4(13)		40±150	1.5	
O + CH_3CH_2CH=CH_2 → products	298	(2.50±0.19)(12)			1.2	280
O + 1-Butene	290-450	8.1(12)	*)	350±100	1.5	
O + cis-CH_3CH=$CHCH_3$ → products	298	(1.06±0.03)(13)			1.1	281
O + cis-2-Butene	290-500	6.6(12)	*)	-140±40	1.5	
O + trans-CH_3CH=$CHCH_3$ → products	298	(1.31±0.12)(13)			1.2	283
O + trans-2-Butene	290-450	1.3(13)	*)	-10±100	1.5	
O + $(CH_3)_2C$=CH_2 → products	298	(1.02±0.06)(13)			1.2	284
O + 1-Propene, 2-methyl-	290-450	9.6(12)	*)	-13±100	1.5	
O + $CH_3CH_2CH_2CH$=CH_2 → products	298	2.8(12)			1.2	285
O + 1-Pentene						

*) For qualifying notes, see this Reaction in the Tables of Kinetic Data.

Index of Reactions and Summary of Recommended Rate Parameters -- Continued

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + cis-CH_3CH=$CHCH_2CH_3$ → products	298	1.0(13)			1.3	285
O + cis-2-Pentene						
O + $(CH_3)_2CHCH$=CH_2 → products	298	2.5(12)			1.2	285
O + 1-Butene, 3-methyl-	290-500	6.0(12)	*)	266	1.5	
O + $(CH_3)_2C$=$CHCH_3$ → products	298	3.4(13)			1.2	286
O + 2-Butene, 2-methyl-	290-400	1.7(13)		-200±200	1.5	
O + $CH_3CH_2CH_2CH_2CH$=CH_2 → products	298	2.8(12)			1.3	286
O + 1-Hexene						
O + $(CH_3)_2C$=$C(CH_3)_2$ → products	298	4.6(13)			1.2	287
O + 2-Butene, 1,2-Dimethyl-	290-550	1.5(13)	*)	-330±100	1.5	
O + cy-CH=$CHCH_2CH_2CH_2$ → products	298	1.27(13)			1.2	288
O + Cyclopentene	290-450	1.43(13)		40±100	1.5	
O + cy-CH=$CHCH_2CH_2CH_2CH_2$ → products	298	1.2(13)			1.2	288
	290-500	1.3(13)		30±200	1.5	
O + Cyclohexene						
O + cy-CH=$C(CH_3)CH_2CH_2CH_2CH_2$ → products	298	5.4(13)			1.2	289
	290-450	1.4(13)		-400±200	1.5	
O + Cyclohexene, 1-methyl-						
O + cy-CH=$CHCH$=$CHCH_2CH_2$ → products	298	5.5(13)			1.2	290
O + 1,3-Cyclohexadiene	290-450	1.4(13)		-400±200	1.5	
O + $C_{10}H_{16}$ → products	298	7.1(13)			1.2	290
O + d-Limonene	290-450	2.7(14)		400±200	1.5	
O + $C_{10}H_{16}$ → products	298	1.7(13)			1.2	291
O + 2-Pinene	290-450	1.9(14)		710±200	1.5	
O + $C_{10}H_{16}$ → products	298	1.6(13)			1.2	291
O + Nopinene	290-450	1.5(14)		660±200	1.5	
O + HALOALKENE and O + KETENE REACTIONS						
O + CH_2=CHF → products	298	(1.96±0.46)(11)			1.2	292
O + Ethene, fluoro-	290-450	5.4(12)		1030±100	1.5	

*) For qualifying notes, see this Reaction in the Tables of Kinetic Data.

Index of Reactions and Summary of Recommended Rate Parameters -- Continued

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + CHF=CHF → products	298	2.7(11)			1.3	293
O + Ethene, 1,2-difluoro-						
O + cis-CHF=CHF → products	298	(1.66±0.48)(11)			1.2	293
O + Ethene, 1,2-difluoro-,(Z)-	290-450	7.2(12)		1170±150	1.5	
O + trans-CHF=CHF → products	298	(2.78±0.61)(11)			1.2	294
O + Ethene, 1,2-difluoro-,(E)-	290-450	8.1(12)		1037±150	1.5	
O + CH_2=CF_2 → products	298	(1.41±0.59)(11)			1.2	294
O + Ethene, 1,1-difluoro-	290-450	4.2(12)		1120±150	1.5	
O + CHF=CF_2 → products	298	(3.45±1.20)(11)			1.2	295
O + Ethene, trifluoro-	290-450	6.1(12)		950±150	1.5	
O + CF_2=CF_2 → products	298	(5.88±1.35)(11)			1.2	296
O + Ethene, tetrafluoro-	290-400	1.6(12)		310±100	1.5	
O + CH_2=CHCl → products	298	(3.85±0.96)(11)			1.2	298
O + Ethene, chloro-	290-450	3.4(12)		670±150	1.5	
O + CH_2=CCl_2 → products	298	5.9(11)			1.2	298
O + Ethene, 1,1-dichloro-						
O + CF_2=CFCl → products	298	3.0(11)			1.2	299
O + Ethene,- 1-chloro-1,2,2-trifluoro-	290-450	2.3(13)		1300±200	1.5	
O + CF_2=CCl_2 → products	298	3.9(11)			1.2	299
O + Ethene, 1,1-dichloro-2,2-difluoro-	290-450	3.5(12)		660±100	1.5	
O + CHCl=CCl_2 → products	298	5.9(10)			1.2	300
O + Ethene, trichloro-						
O + CH_2=CHBr → products	298	(3.78±1.24)(11)			1.3	300
O + Ethene, bromo-	230-449	5.6(12)		835±150	1.5	
O + CH_3CF=CH_2 → products	298	1.2(12)			1.2	300
O + 1-Propene, 2-fluoro-						
O + CH_2FCH=CH_2 → products	298	5.0(11)			1.2	301
O + 1-Propene, 3-fluoro-						
O + CH_3CH=CF_2 → products	298	1.1(12)			1.2	301
O + 1-Propene, 1,1-difluoro-						

Index of Reactions and Summary of Recommended Rate Parameters -- Continued

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + $CF_3CH=CH_2$ → products	298	2.5(10)			1.2	301
O + 1-Propene, 3,3,3-trifluoro-						
O + $CF_3CF=CF_2$ → products	298	1.5(10)			1.2	302
O + 1-Propene,	297-398	7.8(11)		1166±200	1.5	
1,1,2,3,3,3,-hexafluoro-						
O + $CF_2=CFCF=CF_2$ → products	298	2.2(11)			1.2	302
O + 1,3-Butadiene,						
1,1,2,3,4,4-hexafluoro-						
O + $CH_2=CHCH_2Cl$ → products	298	6.1(11)			1.2	303
O + 1-Propene, 3-chloro-						
O + $CH_3C(CF_3)=CH_2$ → products	298	(2.26±0.29)(11)			1.2	303
O + 1-Propene, 2-trifluoromethyl-	200-450	5.8(12)		942±200	1.5	
O + $CH_2FCH_2CH=CH_2$ → products	298	1.4(12)			1.2	304
O + 1-Butene, 4-fluoro-						
O + $CH_3CH_2CF=CF_2$ → products	298	(2.45±0.05)(12)			1.2	304
O + 1-Butene, 1,1,2-trifluoro-						
O + $CH_2=CO$ → adduct(EXV)	298	(2.37±0.79)(11)			1.2	304
O + Ethenone (Ketene)	230-449	1.8(12)		680±200	1.5	
O + $CH_3CH=CO$ → adduct(EXV)	298	(6.8±0.2)(12)			1.2	305
O + 1-Propen-1-one	230-449	2.9(12)		-250±100	1.5	
O + $CH_3CH_2CH=CO$ → adduct(EXV)	298	(7.34±0.84)(12)			1.2	305
O + 1-Buten-1-one	230-449	3.2(12)		-220±100	1.5	
O + $(CH_3)_2C=CO$ → adduct(EXV)	298	(3.0±0.6)(13)			1.2	306
O + 1-Propen-1-one, 2-methyl-	230-449	3.6(12)		-570±100	1.5	
O + ALKYNE REACTIONS						
O + CH≡CH → products	298	9.0(10)			1.2	307
O + Ethyne	250-1300	1.6(13)		1550±100	1.5	
O + CH≡CH → CO + CH_2	300-2500	2.1(12)	1.5	850	2	309
O + Ethyne						
O + CH≡CH → H + CH=C=O	300-600	9.0(12)		2300±300	1.5	309
O + Ethyne	1000-2500	4.3(14)		6100	3	

Index of Reactions and Summary of Recommended Rate Parameters -- Continued

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + CD≡CD → products	298	8.6(10)			1.2	310
O + Ethyne-d2						
O + $CH_3C{\equiv}CH$ → products	298	(4.47±0.41)(11)			1.1	310
O + 1-Propyne	290-1300	1.31(13)		1000±100	1.2	
O + $CH_3C{\equiv}CH$ → H + $[C_3H_3O]^{\cdot}$	298	≤4.3(10)			1.2	311
O + 1-Propyne	295-545	3.6(12)		1320±400	1.5	
Arrhs. Eq. gives upper limits of k.						
O + CH≡CC≡CH → products	298	1.4(12)			1.2	311
O + 1,3-Butadiyne	298-1300	4.5(13)		990±300	1.2	
O + CH_2=CHC≡CH → products	298	1.4(12)			1.2	312
O + 1-Butene-3-yne	298-1300	3.0(13)		910±200	1.5	
O + $CH_3CH_2C{\equiv}CH$ → CO + $CH_3CH{=}CH_2$	298	1.2(12)			1.2	312
O + 1-Butyne	298-1300	2.0(13)		835±100	1.5	
O + $CH_3C{\equiv}CCH_3$ → CO + $CH_3CH{=}CH_2$	298	2.9(12)			1.2	312
O + 2-Butyne	290-360	6(13)		900±300	1.5	
O + $CH_3CH_2CH_2C{\equiv}CH$ → CO(EXV) + $CH_3CH_2CH_2CH$:	298	4.5(11)			1.5	313
O + 1-Pentyne						
O + $CH_3CH_2CH_2CH_2C{\equiv}CH$ → CO(EXV) + $CH_3CH_2CH_2CH_2CH$:	298	3.3(11)			1.5	313
O + 1-Hexyne						
O + AROMATIC HYDROCARBON REACTIONS						
O + C_6H_6 → products	298	(1.22±0.29)(10)			1.3	314
O + Benzene	298-600	1.52(13)		2130±200	2	
O + C_6D_6 → products	298	*)			1.3	315
O + Benzene-d6	376-944	*)		*)	2	
*) Same as for O+C_6H_6						
O + $C_6H_5CH_3$ → products	298	5.0(10)			1.4	315
O + Benzene, methyl-	298-932	1.63(13)		1720±200	2	
O + $C_6H_5CD_3$ → products	298	5.2(10)			1.5	316
O + 1,1,1-trideuterotoluene	298-944	2.2(13)		1800±200	2	

Index of Reactions and Summary of Recommended Rate Parameters -- Continued

Reaction	T/K	k,A $cm^3mol^{-1}s^{-1}$	n	B	k err. factor	Page
O + $C_6H_5CH_2CH_3$ → products	298	6(10)				317
O + Benzene, ethyl-						
O + o-$CH_3C_6H_4CH_3$ → products	298	1.2(11)			1.3	317
O + o-Xylene	298-600	(1.5±1.2)(13)		1382±300	2	
O + o-$CD_3C_6D_4CD_3$ → products	298	1.2(11)			1.3	318
O + o-Xylene-d10	298-600	2.1(13)		1550	2	
O + m-$CH_3C_6H_4CH_3$ → products	298	2.4(11)			1.3	318
O + m-Xylene	298-600	(1.5±1.1)(13)		1216±200	2	
O + m-$CD_3C_6D_4CD_3$ → products	298	2.4(11)			1.3	319
O + m-Xylene-d10	298-600	(1.7±0.4)(13)		1290±80	2	
O + p-$CH_3C_6H_4CH_3$ → products	298	1.2(11)			1.2	319
O + p-Xylene	298-600	(1.57±1.10)(13)		1409±185	2	
O + $C_6H_5C(CH_3)_3$ → products	298	4(10)			2	320
O + Benzene, t-butyl-						
O + 1,2,3-$(CH_3)_3C_6H_3$ → products	298	6.9(11)			1.3	320
O + Benzene, 1,2,3-trimethyl-	298-400	1.0(13)		800±300	2	
O + 1,2,4-$(CH_3)_3C_6H_3$ → products	298	6(11)			1.3	320
O + Benzene, 1,2,4-trimethyl-	298-400	9(12)		800±300	2	
O + 1,3,5-$(CH_3)_3C_6H_3$ → products	298	1.6(12)			2	321
O + Benzene, 1,3,5-trimethyl-	298-600	6.0(12)		400±200	2	
O + C_5H_5N → products	298	4.3(10)			2	321
O + Pyridine	300-500	2.9(12)		1260±300	2	
O + C_6H_5Cl → products	298	3(11)			3	322
O + Benzene, chloro-						
O + C_6H_5F → products	298	8(9)			3	322
O + Benzene, fluoro-						
O + $C_6H_5CF_3$ → products	298	3.5(9)			3	322
O + Benzene, trifluoromethyl-						

4. Tables of Chemical Kinetic Data

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_2{=}CH_2 \rightarrow$ products							
Oxygen atom + Ethene							
58 KAU	EX	296	5(10)				2
Discharge flow-O+NO chemiluminescence.							
Overall k is "about" $5x10^{10}$ cc/mol.sec.							
60 CVE2	RL	298-400	1.01		1011		2/2
k/k_{ref} from products in competing expts.:							
298K: 0.034±0.002; 400K: 0.081±0.006.							
Ref. Rn: O + Cyclopentene → products							
Current normalized values (86 CVE):							
k(298)=4.32(11), A=1.44(13), B=1051.							
60 ELI/SCH	EX	298	(7.23±2.41)(11)				2
Discharge flow-O+NO chemiluminescence.							
P = 0.25-7.5 torr.							
	EX	223-465	(1.1±0.4)(13)		800		2
Discharge flow-O+NO chemiluminescence.							
P = 1.4-2.4 torr.							
63 ELI	EX	298	5.72(11)				2
	EX	223-613	8.4(12)		800		2
Discharge flow-Mass spectrometry							
63 AVR/KOL	EX	313-503	6(10)		680		2
Discharge flow-Final products.							
(Review: 64 AVR/KOL).							
63 AZA/NAL	EX	843-933	1.4(14)		4080±250		2
Ignition limits. An error in Arrh. A							
corrected in 73 HER/HUI.							
67 BRO/THR	EX	298	(3.2±0.4)(11)				2
Discharge flow-ESR. P=1.4-2.8 torr.							
67 TAN/TSU	EX	300	(2.2±1.1)(11)				2
Discharge flow-Mass spectrometry.							
69 NIK/DAB	EX	300	(3.13±0.24)(11)				2
Discharge flow-Mass spec. P=1.0-2.3 torr.							
69 WES/DEH2	EX	298	(4.52±0.30)(11)				2
	EX	195-715	*)	*)	*)		2
Discharge flow-ESR. P=0.9-1.33 torr.							
*) Curved Arrhenius plot. Values of k are:							
195K: (1.44±0.05)(11); 226K: (2.05±0.1)(11);							
273K: (3.3±0.1)(11); 298K: (4.5±0.3)(11);							
381K: (7.4±0.1)(11); 548K: (1.78±0.05)(12);							
555K: (1.96±0.05)(12); 715K: (3.4±0.2)(12).							
71 ATK/CVE	EX	298	(3.00±0.24)(11)				2
Phase shift-O+NO chemiluminescence.							
Updated in 74 FUR/ATK and 76 SIN/CVE.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	'k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CH_2 → products -- Continued							
72 ATK/CVE	EX	298-474	8.1(12)		976±50	2	
Phase shift-O+NO chemiluminescence.							
Updated in 76 SIN/CVE.							
71 STU/NIK	EX	300	(3.79± *))(11)			2	
Flash photolysis-NO+O chemiluminescence.							
*) Stated error limits: +5%, -15%.							
72 STU/NIK	EX	298±2	(3.76±0.38)(11)			2	
Flash photolysis-NO+O and CO+O chemiluminescence.							
72 DAV/HUI	EX	298	5.22(11)			2	
Discharge flow-Mass spectrometry.							
	EX	298	(5.30±0.27)(11)			2	
Flash photolysis-Kinetic absorption.							
	EX	298	(5.08±0.30)(11)			2	
Flash photolysis-Resonance fluorescence.							
	EX	232-500	(3.26±0.18)(12)		569±16	2	
Flash photolysis-Resonance fluorescence.							
73 KUR/HUI	EX	298	(4.79±0.48)(11)			2	
Flash photolysis-Resonance fluorescence.							
73 HER/HUI	SE	298	4.9(11)			2	1.2
	SE	200-500	3.3(12)		565	2	1.2
74 FUR/ATK	EX	298	(4.32±0.45)(11)			2	
Phase shift-O+NO chemiluminescence.							
P = 30-90 torr.							
74 ATK/PIT2	EX	300	(4.00±0.40)(11)			2	
Phase shift-O+NO chemiluminescence.							
Error shown is estimated "overall" error.							
74 ATK/PIT1	EX	298-392	3.37(12)		639±100	2	
Phase shift-O+NO chemiluminescence.							
Error shown is estimated "overall" error.							
74 SLA/PRU	EX	298	(4.64±0.22)(11)			2	
Discharge flow-Mass spectrometry.							
P=0.78-2.14 torr.							
74 MCC	RL	298±5	0.042±0.010			2/2	
Ref. Rn: O + Isobutene → products							
k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins.							
O from O_2 photolysis at 184.9 nm.							
Current normalized value (86 CVE): k=4.28(11)							
76 SIN/CVE	EX	298	(4.23±0.10)(11)			2	
	EX	298-486	(6.98±0.89)(12)		845±47	2	
Phase shift-O+NO chemiluminescence.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_2{=}CH_2 \rightarrow$ products -- Continued							
76 MAN/BRA	EX	298	(4.5±0.2)(11)				2
Flash-photolysis. Resonance-fluorescence. P(tot) = 5 torr.							
77 ATK/PIT1	EX	298	(4.58±0.46)(11)				2
	EX	298-439	5.56(12)		742±100		2
Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.							
80 SUG/ISH	EX	296±2	(6.0±1.2)(11)				2
Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.							
82 NIC/RAV	EX	298	(4.32±0.44)(11)				2
	EX	298-500	(7.35±3.73)(12)		870±190		2
Flash-photolysis. Resonance-fluorescence. O generated by flash-photolysis of O_2. [O] ~ (2-4)(10) molec.cm^{-3}. P(Ar)=100 torr. [$CH_2{=}CH_2$] = (0.01-2.0)(15) molec.cm^{-3}.							
Arrhenius plot is linear below 500 K but exhibits a curvature above 500 K. Measured k values above 500 K are: 552K: (1.6±0.2)(12); 695K: (2.4±0.3)(12); 708K: (2.3±0.2)(12); 736K: (2.7±0.3)(12); 811K: (3.0±0.4)(12); 835K: (3.5±0.9)(12); 944K: (4.2±1.2) (12).							
83 FON/MAE	EX	298-736	*)				2
Discharge flow-mass spectrometry with molecular beam sampling. Large excess of O.							
*) Effect of pressure (0.5-5 torr He) on k: Values of kx10^{-11} at 0.5, 2 & 5 torr: At 298K: 4.10±.48; 4.04±.60; 3.79±.18. At 552K: 15.7±0.6; 14.5±0.8; 14.5±0.4. At 736K: 29.5±2.0; 27.7±2.2; 27.7±2.4. Thus, no evidence of "fall-off" found.							
84 CVE/SIN	SE	298	(4.58±0.16)(11)				2
Selected as the mean of a chosen set of data.							
84 PER1	EX	294	(4.55±0.46)(11)				2
	EX	294-820	4.63(12)	0.63	689		2
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=4.59(11) (calcd. from Arrhs. Eq.)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_2{=}CH_2 \rightarrow$ products -- Continued							
84 PER2	EX	260-860	2.87(12)	1.0	523	2	
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=4.96(11) (calcd. from Arrhs. Eq.)							
84 BRO/STU	EX	298	(3.98±0.24)(11)			2	
	EX	197-372	(5.06±1.63)(12)		757±120	2	
O atoms from H_2 laser photolysis of NO, monitored by O+NO chemiluminescence.							
86 CVE	RN	298	(4.32±0.25)(11)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	298-400	1.44(13)		1051	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
	RN	298±5	(4.28±1.02)(11)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
Recommended value of k	RE	298	(4.40±0.56)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	200-500	6.4(12)	*)	800±200	2	1.5
*) Recommended values of A and B for 200-500K assuming linear Arrhenius plot. However, slightly curved plots have been observed (see, for e.g., 69 WES/DEH, 76 SIN/CVE, 82 NIK/RAV).							
$O + CH_2{=}CH_2 \rightarrow CH_3 + CHO$							
A reaction path in $O + CH_2{=}CH_2 \rightarrow$ products (see 84 CVE/SIN and Sections 1.2 and 1.8)							
82 TEM/WAG	RL	298	0.35-0.60			2/2	
Ref. Rn: $O + CH_2{=}CH_2 \rightarrow$ products							
Reaction of O with $CH_2{=}CH_2$ in an isothermal discharge-flow reactor, with He as carrier gas. LMR-spectrometry. P = 0.75-3.0 torr. In the pressure range 0.75-3.0 torr the "branching ratio" of this reaction path (k/k_{ref}) is in the range 0.35-0.60.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_2{=}CH_2$(EXV) → products							
Oxygen atom + Ethene(EXV)							
76 MAN/BRA	RL	298	1.05±0.34			2/2	
Flash photolysis-Resonance fluorescence. Ethene excited by IR laser. P(Tot)=5 torr. The quoted rate is k/k(unexcited ethene). The observed value of 1.05 shows that there is little or no effect of excited vibration since a value of 1.08 is calculated for thermal heating by the laser alone.							
$O + CD_2{=}CD_2$ → products							
Oxygen atom + Ethene-d_4							
72 STU/NIK	EX	298±2	(3.37±0.34)(11)			2	
Flash photolysis-NO+O & CO+O chemiluminescence.							
73 KUR/HUI	EX	298	(4.93±0.49)(11)			2	
Flash photolysis-Resonance fluorescence. An "overall" estimate of the error in k is given as 10%.							
82 NIC/RAV	EX	298	(4.49±0.38)(11)			2	
	EX	298-475	(7.35±3.73)(12)		870±190	2	
Flash-photolysis. Resonance-fluorescence. O generated by flash-photolysis of O_2. [O] ~ (2-4)(10) molec.cm^{-3}. P(Ar)=100 torr [$CD_2{=}CD_2$] = (0.01-2.0)(15) molec.cm^{-3}. Arrhenius plot is linear below 500 K, but exhibits a curvature above 500 K. Measured k values above 500 K are: 523K: (1.5±0.1)(12); 595K: (1.8±0.2)(12); 708K: (2.3±0.2)(12); 811K: (2.6±0.3)(12).							
Recommended value of k	RE	298	4.4(11)			2	1.2
Recommended values of Arrhenius A and B	RE	200-500	6.4(12)	*)	800±200	2	1.5
*) Recommended values of A and B for 200-500K assuming linear Arrhenius plot. However, slightly curved plots have been observed (see, for e.g., 69 WES/DEH, 76 SIN/CVE, 82 NIK/RAV).							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_2{=}C{=}CH_2 \rightarrow$ products							
Oxygen atom + 1,2-Propadiene (Allene)							
77 ATK/PIT2	EX	297	(6.94±0.66)(11)			2	
	EX	297-439	1.23(13)		883±100	2	
Flash-photolysis. NO_2 chemiluminescence. Error in B is "estimated overall" error.							
79 NIP/SIN	EX	298	(7.83±0.17)(11)			2	
	EX	298-574	(1.8±0.3)(13)		941±54	2	
Modulated, Hg-sensitized N_2O decomposition. Phase-shift technique.							
80 ALE/ARU	EX	295-860	1.0(13)		956±100	2	
Resonance-fluorescence. k(298K)=4.0(11) (calcd. from Arrhs. Eq.)							
Recommended value of k	RE	298	7.4(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-500	1.7(13)	*)	930±100	2	1.5
*) Assumed linear Arrhenius plot in the temperature range 290-450K.							
$O + CH_2{=}C{=}CH_2 \rightarrow H + [C_3H_3O]\cdot$							
A path in the rn. $O + CH_2{=}C{=}CH_2 \rightarrow$ products							
80 ALE/ARU	EX	295-860	6.6(12)		1535±150	2	
Resonance-fluorescence. k(298K)=3.8(10) (calcd. from Arrhs. Eq.)							
$O + CH_3CH{=}CH_2 \rightarrow$ products							
Oxygen atom + 1-Propene							
59 CVE	RL	298	0.23			2/2	
k/k_{ref} from products in competing expts. Ref. Rn: O + Isobutene → products Current normalized value (86 CVE): k=2.35(12)							
63 AVR/KOL	EX	313-393	1.72(12)		1510	2	
Discharge flow-Final products. Extrapolated k(298K)=1.1(10). (Review: 64 AVR/KOL).							
71 STU/NIK	EX	300	(2.17± *))(12)			2	
Flash photolysis-NO+O chemiluminescence. *) Stated error limits: +5%, -15%.							
72 HUI/HER1	EX	298	2.40(12)			2	
Flash photolysis-Resonance fluorescence. Also k=2.07(12) at 215K; k=2.27(12) at 257K.							
72 KUR	EX	298	(2.22±0.15)(12)			2	
	EX	298-424	(2.51±0.20)(12)		38±22	2	
Flash photolysis-Resonance fluorescence.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH=CH_2$ → products -- Continued							
73 HER/HUI	SE	298	2.2(12)			2	1.2
	SE	200-500	2.5(12)		38	2	1.2
74 FUR/ATK	EX	298	(2.02±0.17)(12)			2	
Phase shift-O+NO chemiluminescence.							
74 ATK/PIT2	EX	300	(2.01±0.22)(12)			2	
Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.							
74 ATK/PIT1	EX	298-392	2.08(12)		0±150	2	
Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.							
74 MCC	RL	298±5	0.20±0.05			2/2	
Ref. Rn: O + Isobutene → products k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O_2 photolysis at 184.9 nm. Current normalized value (86 CVE): k=2.04(12)							
75 GAF/ATK1	RL	296±2	0.181±0.010			2/2	
Product yields in competing expts. Ref. Rn: O + Cyclopentene → products Normd. k=2.10(12); update (86 CVE) 2.30(12).							
76 SIN/CVE	EX	298	(2.28±0.08)(12)			2	
	EX	298-483	(7.58±0.42)(12)		363±20	2	
Phase shift-O+NO chemiluminescence.							
77 ATK/PIT1	EX	298	(2.69±0.27)(12)			2	
	EX	298-439	6.32(12)		259±100	2	
Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.							
77 MIC/LEE	EX	298	(2.38±0.25)(12)			2	
Discharge flow-Resonance fluorescence. P = 0.78-2.5 torr.							
78 KOH	EX	298	(2.03±0.11)(12)			2	
	EX	200-353	(3.61±0.42)(12)		168±36	2	
O atoms from H_2 laser photolysis of NO, monitored by O+NO chemiluminescence.							
80 SUG/ISH	EX	296±2	(2.83±0.18)(12)			2	
Pulse-radiolysis. Resonance-absorption P = 50-950 torr.							
82 BIE/HAR	EX	298	(2.65±0.36)(12)			2	
Discharge-flow system. Photoionization mass-spec. P(Tot) ~ 2 torr.							
84 CVE/SIN	SE	298	(2.44±0.12)(12)			2	
Selected as the mean of a chosen set of data.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH{=}CH_2$ → products -- Continued							
84 PER1	EX	293	(2.69±0.27)(12)			2	
	EX	258-861	4.42(11)	2.56	-569	2	
O atoms from F_2 excimer laser photolysis (at 157 nm) of O_2 and NO; [O] monitored by NO + O chemiluminescence. Curved Arrhenius plot: k(298K)=2.98(12) (calcd. from Arrhs. Eq.)							
84 BRO/STU	EX	298	(2.17±0.09)(12)			2	
	EX	197-367	(4.52±1.81)(12)		216±36	2	
O atoms from H_2 laser photolysis of NO, monitored by O+NO chemiluminescence.							
86 CVE	RN	298	2.35(12)			2	
Derived from relative k data (59 CVE) using for Isobutene k=1.02(13)							
	RN	298±5	(2.04±0.51)(12)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
	RN	296±2	(2.30±0.13)(12)			2	
Derived from relative k data (75 GAF/ATK1) using for Cyclopentene k=1.27(13)							
Recommended value of k	RE	298	(2.4±0.3)(12)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	6.1(12)	*)	280±100	2	1.5
*) Recommended values of A and B for 290-450K assuming linear Arrhenius plot. However, slightly curved plots have been observed (see, for e.g., 76 SIN/CVE, 84 PER1, 84 PER2).							
O + $CD_3CD{=}CD_2$ → products							
Oxygen atom + 1-Propene-d_6							
84 PER1	EX	285	(2.77±0.28)(12)			2	
	EX	285-817	3.73(11)	2.53	-609	2	
O atoms from F_2 excimer laser photolysis (at 157 nm) of O_2 and NO; [O] monitored by NO + O chemiluminescence. Curved Arrhenius plot: k(298K)=2.88(12) (calcd. from Arrhs. Eq.)							
Recommended value of k	RE	298	2.4(12)			2	1.2

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CHCH=CH_2 → products							
Oxygen atom + 1,3-Butadiene							
60 CVE/DOY	RL	299-400	1.14		103	2/2	
k/k_{ref} from products in competing expts.: 299K: 0.810±0.018; 400K: 0.884±0.011. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=1.03(13), A=1.63(13), B=143							
73 HER/HUI	SE	298	1.2(13)			2	1.3
	SE	298-400	3.4(12)		-380	2	1.3
74 MCC	RL	298±5	0.96±0.35			2/2	
Ref. Rn: O + Isobutene → products k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O_2 photolysis at 184.9 nm. Current normalized value (86 CVE): k=9.79(12)							
77 ATK/PIT2	EX	297	(1.17±0.11)(13)			2	
	EX	297-439	1.36(13)		53±100	2	
Flash-photolysis. NO_2 chemiluminescence. Error in B is "estimated overall" error.							
79 NIP/SIN	EX	299	(1.31±0.04)(13)			2	
Modulated Hg-sensitized N_2O decomposition. Phase-shift technique.							
80 SUG/ISH	EX	296±2	(1.2±0.1)(13)			2	
Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.							
86 CVE	RN	299	(1.03±0.02)(13)			2	
Derived from relative k data (60 CVE/DOY) using for Cyclopentene k=1.27(13).							
	RN	299-400	1.63(13)		143	2	
Derived from relative k's (60 CVE/DOY) using for Cyclopentene A=1.43(13), B=40.							
	RN	298±5	(9.79±3.57)(12)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
Recommended value of k	RE	298	(1.10±0.10)(13)			2	1.2
Recommended values of Arrhenius A and B	RE	290-500	1.4(13)		40±150	2	1.5

Table 4.1. **Data for O(^{3}P) Reactions with Alkenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH_2CH{=}CH_2$ → products							
Oxygen atom + 1-Butene							
60 CVE2	RL	299-399	0.74		404	2/2	
k/k_{ref} from products in competing expts.: 299K: 0.191±0.006; 399K: 0.268±0.011. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=2.43(12), A=1.06(13), B=444							
71 HUI/HER	EX	298	(2.41±0.19)(12)			2	
Flash photolysis-Resonance fluorescence.							
71 HUI/HER	EX	259-493	(8.79±0.90)(12)		382±30	2	
Flash photolysis-Resonance fluorescence.							
72 HUI/HER1	EX	190-491	*)	*)	*)	2	
Flash photolysis-Resonance fluorescence.							
*) Curved Arrhenius plot. Values of $kx10^{-12}$ increase from 1.95(190K) to 3.57(491K). Authors assume two simultaneous processes: O-addition (A=(2.2±1.1)(12); B=25±105) and H-abstraction (A=9.6±5.4)(12); B=990±216)							
73 HER/HUI	SE	298	2.3(12)			2	1.2
	SE	180-500	*)	*)	*)	2	1.2
*) Selected expression for k=f(T): k=2.3(12)exp(-25/T) + 9.6(12)exp(-990/T) (The 1st term is assumed to be addition and the 2nd H-abstraction by O atoms. For contrary views see 84 CVE/SIN).							
74 FUR/ATK	EX	298	(2.40±0.32)(12)			2	
Phase shift-O+NO chemiluminescence. P = 30-50 torr.							
74 MCC	RL	298±5	0.18±0.07			2/2	
Ref. Rn: O + Isobutene → products k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O_2 photolysis at 184.9 nm. Current normalized value (86 CVE): k=1.84(12)							
76 SIN/CVE	EX	298	(2.38±0.06)(12)			2	
	EX	298-484	(7.21±0.44)(12)		332±23	2	
Phase shift-O+NO chemiluminescence.							
77 ATK/PIT1	EX	298	(2.73±0.28)(12)			2	
	EX	298-439	8.37(12)		334±100	2	
Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH_2CH{=}CH_2$ → products -- Continued							
80 SUG/ISH	EX	296±2	(2.8±0.3)(12)			2	
Pulse-radiolysis. Resonance-absorption P = 50-950 torr.							
84 CVE/SIN	SE	298	(2.55±0.07)(12)			2	
Selected as the mean of a chosen data set.							
84 PER2	EX	260-860	4.45(11)	2.34	-528	2	
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=2.62(12) (calcd. from Arrhs. Eq.)							
84 BRO/STU	EX	298	(2.43±0.07)(12)			2	
	EX	197-372	(5.54±1.81)(12)		241±60	2	
O atoms from H_2 laser photolysis of NO, monitored by O+NO chemiluminescence. Curved Arrhenius plot. For T<273K B=186. For T>273K B=403.							
86 CVE	RN	298	(2.43±0.08)(12)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	299-399	1.06(13)		444	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
	RN	298±5	(1.84±0.71)(12)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
Recommended value of k	RE	298	(2.50±0.19)(12)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	8.1(12)	*)	350±100	2	1.5
*) Assumed linear Arrhs. plot for 290-450K. Slightly curved plots are observed (see for e.g. 73 HER/HUI, 76 SIN/CVE, 84 BRO/STU)							
O + cis-$CH_3CH{=}CHCH_3$ → products							
Oxygen atom + cis-2-Butene							
60 CVE1	RL	300	0.801±0.014			2/2	
k/k_{ref} from products in competing expts. Ref. Rn: O + Cyclopentene → products Current normalized value (86 CVE): k=1.02(13)							
73 DAV/HUI	EX	298	(1.03±0.04)(13)			2	
	EX	268-443	(5.84±0.58)(12)		-161±32	2	
Flash photolysis-Resonance fluorescence.							
73 HER/HUI	SE	298	1.0(13)			2	
	SE	200-500	5.9(12)		-165	2	1.2

Table 4.1. Data for O(^{3}P) Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + cis-$CH_3CH{=}CHCH_3$ → products -- Continued							
74 FUR/ATK	EX	298	(9.00±1.76)(12)			2	
Phase shift-O+NO chemiluminescence. P = 30-50 torr.							
74 MCC	RL	298±5	0.79±0.25			2/2	
Ref. Rn: O + Isobutene → products k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O_2 photolysis at 184.9 nm. Current normalized value (86 CVE): k=8.06(12)							
76 SIN/CVE	EX	298	(1.06±0.04)(13)			2	
	EX	298-484	(6.68±0.23)(12)		-135±13	2	
Phase shift-O+NO chemiluminescence.							
77 ATK/PIT1	EX	298	(1.09±0.11)(13)			2	
	EX	298-439	7.29(12)		-118±100	2	
Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.							
80 SUG/ISH	EX	296±2	(1.2±0.2)(13)			2	
Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.							
84 CVE/SIN	SE	298	(1.06±0.02)(13)			2	
Selected as the mean of a chosen set of data.							
84 PER2	EX	260-860	5.66(11)	2.07	-881	2	
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=1.09(13) (calcd. from Arrhs. Eq.)							
86 CVE	RN	300	(1.02±0.02)(13)			2	
Derived from relative k data (60 CVE1) using for Cyclopentene k=1.27(13).							
	RN	298±5	(8.06±2.55)(12)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
Recommended value of k	RE	298	(1.06±0.03)(13)			2	1.1
Recommended values of Arrhenius A and B	RE	290-500	6.6(12)	*)	-140±40	2	1.5
*) Assumed linear Arrhs. plot for 290-500K. Slightly curved plots are observed (see for e.g. 76 SIN/CVE, 84 PER2)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + trans-$CH_3CH=CHCH_3$ → products							
Oxygen atom + trans-2-Butene							
60 CVE1	RL	300	0.951±0.042			2/2	
k/k_{ref} from products in competing expts.							
Ref. Rn: O + Cyclopentene → products							
Current normalized value (86 CVE): k=1.21(13)							
73 HER/HUI	SE	298	1.4(13)			2	1.3
74 MCC	RL	298±5	1.25±0.3			2/2	
Ref. Rn: O + Isobutene → products							
k/k_{ref} obtained from ratios of NO+O chemi-luminescence signals with different olefins.							
O from O_2 photolysis at 184.9 nm.							
Current normalized value (86 CVE): k=1.28(13)							
77 ATK/PIT1	EX	298	(1.42±0.14)(13)			2	
	EX	298-439	1.36(13)		-10±100	2	
Flash photolysis-Chemiluminescence.							
Error in B is "estimated overall" error.							
80 SUG/ISH	EX	296±2	(1.4±0.2)(13)			2	
Pulse-radiolysis. Resonance-absorption							
P = 50-950 torr.							
84 CVE/SIN	SE	298	(1.34±0.08)(13)			2	
Selected as the mean of a chosen set of data.							
84 PER2	EX	260-860	5.78(11)	2.17	-906	2	
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot.							
k(298K)=1.21(13) (calcd. from Arrhs. Eq.)							
86 CVE	RN	300	(1.21±0.05)(13)			2	
Derived from relative k data (60 CVE1) using for Cyclopentene k=1.27(13).							
	RN	298±5	(1.28±0.36)(13)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							
Recommended value of k	RE	298	(1.31±0.12)(13)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	1.3(13)	*)	-10±100	2	1.5
*) Assumed linear Arrhs. plot for 290-450K. Slightly curved plots are observed (see for e.g. 76 SIN/CVE, 84 PER2)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + (CH_3)_2C{=}CH_2 \rightarrow$ products							
Oxygen atom + 1-Propene, 2-methyl- (Isobutene)							
60 CVE2	RL	299-403	0.67		-65	2/2	
k/k_{ref} from products in competing expts.: 299K: 0.838±0.020; 403K: 0.792±0.011. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=1.06(13), A=9.58(12), B=-25							
73 HER/HUI	SE	298	1.2(13)			2	1.3
Selected value 1973.							
74 FUR/ATK	EX	298	(9.85±1.34)(12)			2	
Phase shift-O+NO chemiluminescence. P = 30-50 torr.							
76 SIN/CVE	EX	298	(1.04±0.03)(13)			2	
	EX	298-484	(8.74±0.53)(12)		-51±22	2	
Phase shift-O+NO chemiluminescence.							
77 ATK/PIT1	EX	298	(9.22±0.90)(12)			2	
	EX	298-439	1.06(13)		43±100	2	
Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.							
80 SUG/ISH	EX	296±2	(1.0±0.1)(13)			2	
Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.							
84 CVE/SIN	SE	298	(1.03±0.06)(13)			2	
Selected as the mean of a chosen set of data.							
84 PER2	EX	260-860	7.11(11)	2.11	-805	2	
O atoms from F_2 excimer laser photolysis (157 nm) of O_2 & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=1.06(13) (calcd. from Arrhs. Eq.) Curved Arrhenius plot.							
86 CVE	RN	299	(1.06±0.03)(13)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	299-403	9.58(12)		-25	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	(1.02±0.06)(13)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	9.6(12)	*)	-13±100	2	1.5
*) Assumed linear Arrhs. plot for 290-450K. Slightly curved plots are observed (see for e.g. 76 SIN/CVE, 84 PER2)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH_2CH_2CH{=}CH_2$ → products							
Oxygen atom + 1-Pentene							
57 FOR/END	RN	300±3	(2.85±0.71)(12)			2	
Relative rate placed by the authors on absolute scale using k(O+O_2+M) of 55 BEN/AXW. O-atoms from NO2 photolysis at 366 nm.							
73 HER/HUI	SE	298	2.8(12)			2	1.3
82 BIE/HAR	EX	298	(2.83±0.30)(12)			2	
Discharge-flow system. Photoionization mass-spectrometry. P(Tot) ~ 2 torr.							
Recommended value of k	RE	298	2.8(12)			2	1.2
O + cis-$CH_3CH{=}CHCH_2CH_3$ → products							
Oxygen atom + cis-2-Pentene							
57 FOR/END	RN	300±3	(1.09±0.10)(13)			2	
Relative rate placed by the authors on absolute scale using k(O+O_2+M) of 55 BEN/AXW. O-atoms from NO2 photolysis at 366 nm.							
59 CVE	RL	298	0.75			2/2	
k/k_{ref}: from products in competing expts. Ref. Rn: O + Cyclopentene → products Current normalized value (86 CVE): k=9.5(12)							
73 HER/HUI	SE	298	1.1(13)			2	1.3
86 CVE	RN	298	9.5(12)			2	
Derived from relative k data (59 CVE) using for Cyclopentene k=1.27(13).							
Recommended value of k	RE	298	1.0(13)			2	1.3
O + $(CH_3)_2CHCH{=}CH_2$ → products							
Oxygen atom + 1-Butene, 3-methyl-							
74 MCC	RL	298±5	0.22±0.05			2/2	
Ref. Rn: O + Isobutene → products k/k_{ref} obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O_2 photolysis at 184.9 nm. Current normalized value (86 CVE): k=2.24(12)							
76 SIN/CVE	EX	298	(2.53±0.04)(12)			2	
	EX	298-484	(6.02±0.44)(12)		266±26	2	
Phase shift-O+NO chemiluminescence.							
86 CVE	RN	298±5	(2.24±0.51)(12)			2	
Derived from relative k data (74 MCC) using for Isobutene k=1.02(13)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $(CH_3)_2CHCH{=}CH_2$ → products -- Continued							
Recommended value of k	RE	298	2.5(12)			2	1.2
Recommended values of Arrhenius A and B	RE	290-500	6.0(12)	*)	266	2	1.5
*) Assumed linear Arrhs. plot for 290-450K. Slightly curved plots are observed (see for e.g. 76 SIN/CVE)							
O + $(CH_3)_2C{=}CHCH_3$ → products							
Oxygen atom + 2-Butene, 2-methyl-							
60 CVE2	RL	298-400	1.18		-240	2/2	
k/k_{ref} from products in competing expts.: 299K: 2.66±0.07; 400K: 2.19±0.09. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=3.38(13), A=1.69(13), B=-200							
73 HER/HUI	SE	298	3.8(13)			2	1.3
	SE	298-400	3.9(12)		-680	2	1.3
74 FUR/ATK	EX	298	(3.1±0.3)(13)			2	
Phase shift-O+NO chemiluminescence. P = 30-50 torr.							
80 SUG/ISH	EX	296±2	(3.3±0.3)(13)			2	
Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.							
84 CVE/SIN	SE	298	(3.32±0.22)(13)			2	
Selected as the mean of a chosen set of data.							
86 CVE	RN	299	(3.38±0.09)(13)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	298-400	1.69(13)		-200	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	3.4(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-400	1.7(13)		-200±200	2	1.5
O + $CH_3CH_2CH_2CH_2CH{=}CH_2$ → products							
Oxygen atom + 1-Hexene							
60 CVE1	RL	299	0.218±0.004			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + Cyclopentene → products Current normalized value (86 CVE): k=2.77(12)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH_2CH_2CH_2CH=CH_2$ → products -- Continued							
73 HER/HUI	SE	298	3.1(12)			2	1.3
86 CVE	RN	299	(2.77±0.05)(12)			2	
Derived from relative k data (60 CVE1) using for Cyclopentene k=1.27(13).							
Recommended value of k	RE	298	2.8(12)			2	1.3
O + $(CH_3)_2C=C(CH_3)_2$ → products							
Oxygen atom + 2-Butene, 1,2-Dimethyl- (Tetramethylethylene)							
60 CVE2	RL	300-393	1.25		-300	2/2	
k/k_{ref} from products in competing expts.: 300K: 3.41±0.02; 393K: 2.69±0.14. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=4.33(13), A=1.79(13), B=-260							
73 HER/HUI	SE	298	4.8(13)			2	1.2
	SE	298-400	3.4(12)		-790	2	1.2
73 DAV/HUI	EX	298	(4.77±0.18)(13)			2	
	EX	290-355	(3.36±0.64)(12)		-790±60	2	
Flash photolysis-Resonance fluorescence.							
74 FUR/ATK	EX	298	(4.44±0.41)(13)			2	
Phase shift-O+NO chemiluminescence. P = 30-50 torr.							
75 SIN/FUR	EX	298	(4.58±0.10)(13)			2	
	EX	298-481	(1.24±0.12)(13)		-390±38	2	
Phase shift-O+NO chemiluminescence.							
84 CVE/SIN	SE	298	(4.63±0.07)(13)			2	
Selected as the mean of a chosen set of data.							
86 CVE	RN	300	(4.33±0.03)(13)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	300-393	1.79(13)		-260	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	4.6(13)			2	1.2
Recommended values of Arrhenius A and B	RE	290-550	1.5(13)	*)	-330±100	2	1.5
*) Assumed linear Arrhs. plot for 290-450K. Slightly curved plots are observed (see for e.g. 76 SIN/CVE)							

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + cy-CH=CHCH$_2$CH$_2$CH$_2$ → products							
Oxygen atom + Cyclopentene							
60 CVE2	RL	299-403	1.49		65	2/2	
k/k_{ref} from products in competing expts.: 299K: 1.19±0.028; 403K: 1.26±0.018. Ref. Rn: O + Isobutene → products Current normalized values (86 CVE): k(298)=1.21(13), A=1.43(13), B=52							
73 HER/HUI	SE	298	1.4(13)			2	1.3
	SE	298-400	3.3(12)		-430	2	1.3
75 GAF/ATK2	RL	296-423	2.33		-252±40	2/2	
k/k_{ref} from products in competing expts.: 296K: 5.52±0.31; 333K: 4.93±0.63; 373K: 4.44±0.38; 423K: 4.33±0.22. Ref. Rn: O + 1-Propene → products See also 75 GAF/ATK1. Normalized values: A=5.6(12), B=-216±40; updates (86 CVE): A=1.4(13), B=28, k(298)=1.3(13) (86 CVE)							
86 CVE	RN	298	(1.21±0.03)(13)			2	
Derived from relative k data (60 CVE2) using $k_{iso\text{-}Butene}$ = 1.02(13) .							
	RN	299-403	1.43(13)		52	2	
Derived from relative k data (60 CVE2) using for iso-Butene A=9.6(12), B=-13.							
	RN	296	(1.32±0.07)(13)			2	
Derived from relative k data (75 GAF/ATK2) using $k_{Propene}$ = 2.4(12) .							
	RN	296-423	(1.42±0.47)(13)		28±140	2	
Derived from relative k data (75 GAF/ATK2). using for Propene A=6.1(12), B=280.							
Recommended value of k	RE	298	1.27(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	1.43(13)		40±100	2	1.5
O + cy-CH=CHCH$_2$CH$_2$CH$_2$CH$_2$ → products							
Oxygen atom + Cyclohexene							
60 CVE2	RL	298-400	0.89		-7	2/2	
k/k_{ref} from products in competing expts.: 299K: 0.907±0.044; 399K: 0.902±0.064. Ref. Rn: O + Cyclopentene → products Current normalized values (86 CVE): k(298)=1.15(13), A=1.3(13), B=33							
73 HER/HUI	SE	298	1.3(13)			2	1.3
	SE	298-400	2.8(12)		-460	2	1.3

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + cy-CH=CHCH$_2$CH$_2$CH$_2$CH$_2$ → products -- Continued							
82 WAS/TAK Reaction of Cyclohexene with O atoms in a fast-flow reactor. O atoms generated by a microwave-discharge in a He-O_2 mixture. Mass-spectrometry. P(Tot) = 3.7 torr. P(Cyclohexene) = 0.004-0.012 mtorr. P$(O_2)_o$ = 0.266-0.560 mtorr.	EX	298	(1.20±0.03)(13)			2	
86 CVE Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).	RN	298	(1.15±0.06)(13)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.	RN	298-400	1.27(13)		33	2	
Recommended value of k	RE	298	1.2(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-500	1.3(13)		30±200	2	1.5
O + cy-CH=C(CH$_3$)CH$_2$CH$_2$CH$_2$CH$_2$ → products							
Oxygen atom + Cyclohexene, 1-methyl-							
75 GAF/ATK2 k/k_{ref} from products in competing expts.: 296K: 4.21±0.17; 333K: 3.93±0.25; 373K: 3.22±0.32; 423K: 2.71±0.27. Ref. Rn: O + Cyclopentene → products Normalized A=5.3(12), B=-669±111; updates: A=1.36(13), B=-413, k(298)=5.4(13) (86 CVE)	RL	296-423	0.95		-453±70	2/2	
86 CVE Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).	RN	296	(5.35±0.22)(13)			2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13), B=40.	RN	296-423	1.36(13)		-413	2	
Recommended value of k	RE	298	5.4(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	1.4(13)		-400±200	2	1.5

Table 4.1. Data for $O(^3P)$ Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + cy-CH=CHCH=CHCH$_2$CH$_2$ → products							
Oxygen atom + 1,3-Cyclohexadiene							
75 GAF/ATK2	RL	296-423	0.92		-448±55	2/2	
k/k_{ref} from products in competing expts.: 296K: 4.33±0.20; 333K: 3.43±0.24; 373K: 3.05±0.31; 423K: 2.74±0.27. Ref. Rn: O + Cyclopentene → products Normalized A=5.1(12), B=-664±91; updates: A=1.32(13), B=-408, k(298)=5.5(13) (86 CVE)							
86 CVE	RN	296	(5.50±0.25)(13)			2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).							
	RN	296-423	1.32(13)		-408	2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	5.5(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	1.4(13)		-400±200	2	1.5
O + $C_{10}H_{16}$ → products							
Oxygen atom + d-Limonene (Cyclohexene, 1-methyl-4-(1-methylethenyl)-,(R))							
75 GAF/ATK2	RL	296-423	19.63		362±35	2/2	
k/k_{ref} from products in competing expts.: 296K: 5.61±0.45; 333K: 6.74±0.50; 373K: 7.45±0.45; 423K: 8.16±0.57. Ref. Rn: O + Cyclopentene → products Normalized A=1.1(14), B=151±75; updates: A=2.81(14), B=402, k(298)=7.1(13) (86 CVE)							
86 CVE	RN	296	(7.12±0.57)(13)			2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).							
	RN	296-423	2.81(14)		402	2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	7.1(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	2.7(14)		400±200	2	1.5

Table 4.1. **Data for O(^{3}P) Reactions with Alkenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $C_{10}H_{16}$ → products							
Oxygen atom + 2-Pinene							
(Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-)							
75 GAF/ATK2	RL	296-423	13.46		674±30	2/2	
k/k_{ref} from products in competing expts.: 296K: 1.38±0.05; 333K: 1.84±0.09; 373K: 2.22±0.15; 423K: 2.73±0.27. Ref. Rn: O + Cyclopentene → products Normalized A=7.5(13), B=458±70; updates: A=1.92(14), B=714, k(298)=1.75(13) (86 CVE)							
86 CVE	RN	296	(1.75±0.06)(13)			2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).							
	RN	296-423	1.92(14)		714	2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13). B=40.							
Recommended value of k	RE	298	1.7(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	1.9(14)		710±200	2	1.5
O + $C_{10}H_{16}$ → products							
Oxygen atom + Nopinene							
(Bicyclo[3.1.1]heptene, 6,6-dimethyl-methylene-)							
75 GAF/ATK2	RL	296-423	10.77		619±30	2/2	
k/k_{ref} from products in competing expts.: 296K: 1.30±0.05; 333K: 1.64±0.11; 373K: 2.07±0.20; 423K: 2.41±0.12. Ref. Rn: O + Cyclopentene → products Normalized A=6.0(13), B=413±70; updates: A=1.54(14), B=659, k(298)=1.65(14) (86 CVE)							
86 CVE	RN	296	(1.65±0.06)(13)			2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).							
	RN	296-423	1.54(14)		659	2	
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	298	1.6(13)			2	1.2
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.	RE	290-450	1.5(14)		660±200	2	1.5

Table 4.2. **Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes**

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CHF → products							
Oxygen atom + Ethene, fluoro- (Fluoroethylene)							
71 MOS	RL	296	0.38			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.9(11) (73 HER/HUI). Current update (86 CVE) k=1.67(11)							
72 HUI/HER2	EX	307	(2.63±0.38)(11)			2	
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	2.6(11)			2	1.3
74 JON/MOS	RL	298-420	0.94		243	2/2	
k/k_{ref} from products in competing expts.: 298K: 0.409; 420K: 0.516. Ref. Rn: O + CH_2=CH_2 → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=1.80(11), A=6.02(12), B=1043							
75 SLA/GUT	EX	302±2	2.47(11)			2	
Discharge fast-flow reactor-Photoionization mass spec. Measured 1st order olefin concn. decay. k superseded by data in 84 PAR/SAW2.							
76 ATK/PIT	EX	298±2	(1.61±0.20)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decompn. of N_2O.							
81 SUG/OKA	EX	298±2	3.13(11)			2	
Pulse radiolysis-Resonance absorption.							
84 PAR/SAW2	EX	300±3	(2.07±0.11)(11)			2	
Fast-flow reactor-Photoionization mass spec. Quoted error is 1σ; estimd. accuracy: ±20%. At P=0.6-3.5 torr, k is P invariant (±20%).							
77 ATK/PIT3	EX	298-442	4.84(12)		1019±100	2	
k(298K): (1.59±0.16)(11). Flash photolysis-O+NO chemiluminescence.							
86 CVE	RN	296	1.67(11)			2	
Derived from relative k (71 MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298	1.80(11)			2	
Derived from relative k (74 JON/MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298-420	6.02(12)		1043	2	
Derived from relative k's (74 JON/MOS) using for CH_2=CH_2 A=6.40(12), B=800.							

Table 4.2. **Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CHF → products -- Continued							
Recommended value of k	RE	298	(1.96±0.46)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	5.4(12)		1030±100	2	1.5
O + CHF=CHF → products							
Oxygen atom + Ethene, 1,2-difluoro-							
72 HUI/HER2	EX	307	(2.70±0.34)(11)			2	
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	2.7(11)			2	1.3
Recommended value of k	RE	298	2.7(11)			2	1.3
O + cis-CHF=CHF → products							
Oxygen atom + Ethene, 1,2-difluoro-,(Z)-							
71 MOS	RL	296	0.32			2/2	
k/k_{ref} from products in competing expts.:							
Ref. Rn: O + CH_2=CH_2 → products							
O from Hg-photosensitized decompn. of N_2O.							
Normalized absolute k=1.5(11) (73 HER/HUI).							
Current update (86 CVE) k=1.41(11)							
74 JON/MOS	RL	298-420	1.12		373	2/2	
k/k_{ref} from products in competing expts.:							
298K: 0.309; 420K: 0.452.							
Ref. Rn: O + CH_2=CH_2 → products							
Measured: epoxide & aldehyde from Ref. Rn.							
O from Hg-photosensitized decompn. of N_2O.							
Current normalized values (86 CVE):							
k(298)=1.36(11), A=7.17(12), B=1173							
76 GIL/SLA	EX	300±2	2.22(11)			2	
Discharge fast-flow reactor-Photoionization mass spec. k's from 1st order decay of olefin concn. Estimated accuracy: ±20%.							
86 CVE	RN	296	1.41(11)			2	
Derived from relative k (71 MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298	1.36(11)			2	
	RN	298-420	7.17(12)		1173	2	
Derived from relative k's (74 JON/MOS) using for CH_2=CH_2 k(298)=4.40(11), A=6.40(12), B=800.							
Recommended value of k	RE	298	(1.66±0.48)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	7.2(12)		1170±150	2	1.5

Table 4.2. Data for O(^{3}P) Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + trans-CHF=CHF → products							
Oxygen atom + Ethene, 1,2-difluoro-,(E)-							
71 MOS	RL	296	0.54			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.6(11) (73 HER/HUI). Current update (86 CVE) k=2.38(11)							
74 JON/MOS	RL	298-420	1.27		237	2/2	
k/k_{ref} from products in competing expts.: 298K: 0.564; 420K: 0.713. Ref. Rn: O + CH_2=CH_2 → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=2.48(11), A=8.1(12), B=1037							
76 GIL/SLA	EX	300±2	3.49(11)			2	
Discharge fast-flow reactor-Photoionization mass spec. k's from 1st order decay of olefin concn. Estimated accuracy: ±20%.							
86 CVE	RN	296	2.38(11)			2	
Derived from relative k (71 MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298	2.48(11)			2	
Derived from relative k (74 JON/MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298-420	8.1(12)		1037	2	
Derived from relative k's (74 JON/MOS) using for CH_2=CH_2 A=6.40(12), B=800.							
Recommended value of k	RE	298	(2.78±0.61)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	8.1(12)		1037±150	2	1.5
O + CH_2=CF_2 → products							
Oxygen atom + Ethene, 1,1-difluoro-							
71 MOS	RL	296	0.22			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.1(11) (73 HER/HUI). Current update (86 CVE) k=9.68(10)							
72 HUI/HER2	EX	307	(2.19±0.18)(11)			2	
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	2.2(11)			2	1.3

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CF_2 → products -- Continued							
74 JON/MOS	RL	298-420	0.65		321	2/2	
k/k_{ref} from products in competing expts.: 298K: 0.215; 420K: 0.299. Ref. Rn: O + CH_2=CH_2 → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=9.46(10), A=4.16(12), B=1121							
76 GIL/SLA	EX	300±2	1.87(11)			2	
Discharge fast-flow reactor-Photoionization mass spec. k's from 1st order decay of olefin concn. Estimated accuracy: ±20%.							
81 SUG/OKA	EX	298±2	1.20(11)			2	
Pulse radiolysis-Resonance absorption.							
86 CVE	RN	296	9.68(10)			2	
Derived from relative k (71 MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	298	9.46(10)			2	
Derived from relative k (74 JON/MOS) using for CH_2=CH_2 k=4.40(11).							
	RN	290-450	4.16(12)		1121	2	
Derived from relative k's (74 JON/MOS) using for CH_2=CH_2 A=6.40(12), B=800.							
Recommended value of k	RE	298	(1.41±0.59)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	4.2(12)		1120±150	2	1.5
O + CHF=CF_2 → products							
Oxygen atom + Ethene, trifluoro-							
71 MOS	RL	296	0.57			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.7(11) (73 HER/HUI). Current update (86 CVE) k=2.51(11)							
74 JON/MOS	RL	298-420	0.96		147	2/2	
k/k_{ref} from products in competing expts.: 298K: 0.569; 420K: 0.569. Ref. Rn: O + CH_2=CH_2 → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=2.50(11), A=6.14(12), B=947							

Table 4.2. Data for $O(^3P)$ Reactions with Halpalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CHF=CF_2$ → products -- Continued							
76 GIL/SLA Discharge fast-flow reactor-Photoionization mass spec. k's from 1st order decay of olefin concn. Estimated accuracy: ±20%.	EX	300±2	5.00(11)			2	
81 SUG/OKA Pulse radiolysis-Resonance absorption.	EX	298±2	3.79(11)			2	
86 CVE Derived from relative k (71 MOS) using for $CH_2=CH_2$ k=4.40(11).	RN	296	2.51(11)			2	
Derived from relative k (74 JON/MOS) using for $CH_2=CH_2$ k=4.40(11).	RN	298	2.50(11)			2	
Derived from relative k's (74 JON/MOS) using for $CH_2=CH_2$ A=6.40(12), B=800.	RN	298-420	6.14(12)		947	2	
Recommended value of k	RE	298	(3.45±1.20)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	6.1(12)		950±150	2	1.5
O + $CF_2=CF_2$ → products							
Oxygen atom + Ethene, tetrafluoro-							
65 SAU/HEI1 k/k_{ref} from products in competing expts. Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=5.0(11) (73 HER/HUI). Current update (86 CVE) k=4.54(11)	RL	297	1.031			2/2	
66 SAU/HEI *) k/k_{ref} from products in competing expts: 1.10(297K), 0.856(343K), 0.735(398K) Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normd. k(298)=5.3(11) (73 HER/HUI); updates: k(298)=4.84(11), A=1.43(12), B=322 (86 CVE).	RL	297-398	*)		*)	2/2	
69 TYE k/k_{ref} from products in competing expts.: Ref. Rn: O + $CH_2=CH_2$ → products O from flash photolysis of NO_2. CF_2 monitored by kinetic spectroscopy. Normalized absolute k=5.0(11) (73 HER/HUI). Current update (86 CVE) k=4.62(11)	RL	296	1.05±0.05			2/2	

Table 4.2. **Data for O(^{3}P) Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CF_2=CF_2 → products -- Continued							
71 MOS	RL	296	1.60			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=9.1(11) (73 HER/HUI). Current update (86 CVE) k=7.04(11)							
73 HER/HUI	SE	298	5(11)			2	1.4
	SE	298-500	7.7(11)		100	2	1.4
74 JON/MOS	RL	298-420	0.78		-245	2/2	
k/k_{ref} from products in competing expts. 298K: 1.707; 420K: 1.338. Ref. Rn: O + CH_2=CH_2 → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=7.51(11), A=4.98(12), B=555							
75 GER/MOI	RL	300-406	0.11±0.06		-1258±20	2/2	
k/k_{ref} from products in competing expts. using a modified "diffusion flame" method: Ref. Rn: O + CH≡CH → products Taken k_{ref}=2(13)exp(-1610/T) & obtained k(298K)=7.02(11); A=2.29(12); B=352.							
79 KOD	EX	298±5	(4.28±0.12)(11)			2	
From decay of $CF_2(^3B_1)$ emission. O from Hg-photosensitized decompn. of N_2O.							
81 SUG/OKA	EX	298±2	4.88(11)			2	
Pulse radiolysis-Resonance absorption.							
86 CVE	RN	297	4.54(11)			2	
Derived from relative k (65 SAU/HEI1) using for CH_2=CH_2 k=4.40(11).							
	RN	297	4.84(11)			2	
Derived from relative k (66 SAU/HEI) using for CH_2=CH_2 k=4.40(11).							
	RN	297-398	1.43(12)		322±100	2	
Derived from relative k's (66 SAU/HEI) using for CH_2=CH_2 A=6.40(12), B=800.							
	RN	296	4.62(11)			2	
Derived from relative k (69 TYE) using for CH_2=CH_2 k=4.40(11).							
	RN	296	7.04(11)			2	
Derived from relative k (71 MOS) using for CH_2=CH_2 k=4.40(11).							

Table 4.2. **Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CF_2=CF_2 → products -- Continued							
86 CVE	RN	298	7.51(11)			2	
	RN	298-420	4.99(11)		555	2	
Derived from relative k's (74 JON/MOS) using for CH_2=CH_2 k(298)=4.40(11), A=6.40(12), B=800.							
	RN	298	6.70(11)			2	
	RN	300-406	1.71(12)		292	2	
Derived from relative k's (75 GER/MOI) using for Acetylene k(298)=8.6(10), A=1.55(13), B=1550.							
Recommended value of k	RE	298	(5.88±1.35)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-400	1.6(12)		310±100	2	1.5
O + CH_2=$CHCl$ → products							
Oxygen atom + Ethene, chloro- (Chloroethylene)							
72 HUI/HER2	EX	307	(5.22±0.24)(11)			2	
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	5.2(11)			2	1.3
75 SLA/GUT	EX	302±2	3.79(11)			2	
Discharge fast-flow reactor coupled to a photoionization mass spectrometer. Measured the 1st order decay of olefin concentration.							
76 ATK/PIT	EX	298±2	(2.54±0.26)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decompn. of N_2O.							
77 WES/DEH	EX	297	(4.1±0.1)(11)			2	
Flash photolysis-Resonance fluorescence.							
77 ATK/PIT3	EX	298-442	3.36(12)		667±100	2	
K(298K): (3.60±0.36)(11). Flash photolysis-O+NO chemiluminescence.							
Recommended value of k	RE	298	(3.85±0.96)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	3.4(12)		670±150	2	1.5
O + CH_2=CCl_2 → products							
Oxygen atom + Ethene, 1,1 dichloro-							
75 SAN/HEI	RL	298	1.0			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CF_2=CF_2 → products Measured: CO and CF_2O from Ref. Rn. O from Hg-photosensitized decompn. of N_2O. Current normalized k=5.88(11) (86 CVE).							

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CCl_2 → products -- Continued							
86 CVE	RN	298	5.88(11)			2	
Derived from relative k (75 SAN/HEI) using for CF_2=CF_2 k=5.88(11).							
Recommended value of k	RE	298	5.9(11)			2	1.2
O + CF_2=$CFCl$ → products							
Oxygen atom + Ethene, 1-chloro-1,2,2-trifluoro-							
69 TYE	RL	296-419	14.4		989	2/2	
k/k_{ref} from products in competing expts.: 0.51(296K), 1.36(419K)							
Ref. Rn: O + CF_2=CF_2 → products							
O from flash photolysis of NO_2. CF_2 monitored by kinetic spectroscopy.							
Current normalized values (86 CVE): k(298)=3.00(11), A=2.26(12), B=1296.							
86 CVE	RN	296	3.00(11)			2	
	RN	296-419	2.26(13)		1296	2	
Derived from relative k's (69 TYE) using for CF_2=CF_2 k(298)=5.88(11), A=1.57(12), B=307.							
Recommended value of k	RE	298	3.0(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	2.3(13)		1300±200	2	1.5
O + CF_2=CCl_2 → products							
Oxygen atom + Ethene, 1,1-dichloro-2,2-difluoro-							
69 TYE	RL	296-419	2.20		352	2/2	
k/k_{ref} from products in competing expts.: 0.67(296K), 0.95(419K)							
Ref. Rn: O + CF_2=CF_2 → products							
O from flash photolysis of NO_2. CF_2 monitored by kinetic spectroscopy.							
Current normalized values (86 CVE): k(298)=3.94(11), A=3.45(12), B=659.							
86 CVE	RN	296	3.94(11)			2	
	RN	296-419	3.45(12)		659	2	
Derived from relative k's (69 TYE) using for CF_2=CF_2 k(298)=5.88(11), A=1.57(12), B=307.							
Recommended value of k	RE	298	3.9(11)			2	1.2
Recommended values of Arrhenius A and B	RE	290-450	3.5(12)		660±100	2	1.5

Table 4.2. **Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CHCl=CCl_2$ → products							
Oxygen atom + Ethene, trichloro-							
74 SAN/HEI	RL	298	0.10			2/2	
k/k_{ref} from CO yields in competing expts., O from Hg-photosensitized decompn. of N_2O. Ref. Rn: O + $CF_2=CF_2$ → products Current normalized k=5.88(11) (86 CVE).							
86 CVE	RN	298	5.88(10)			2	
Derived from relative k (74 SAN/HEI) using for $CF_2=CF_2$ k=5.88(10).							
Recommended value of k	RE	298	5.9(10)			2	1.2
O + $CH_2=CHBr$ → products							
Oxygen atom + Ethene, bromo- (Bromoethylene)							
72 HUI/HER2	EX	307	(4.90±0.34)(11)			2	
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	4.9(11)			2	1.3
75 SLA/GUT	EX	302±2	3.98(11)			2	
Discharge fast-flow reactor coupled to a photoionization mass spectrometer. Measured the 1st order decay of olefin concentration.							
76 ATK/PIT	EX	298±2	(2.45±0.25)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decompn. of N_2O.							
77 ATK/PIT3	EX	298-442	5.63(12)		835±100	2	
k(298K): (3.40±0.34)(11). Flash photolysis-O+NO chemiluminescence.							
Recommended value of k	RE	298	(3.78±1.24)(11)			2	1.3
Recommended values of Arrhenius A and B	RE	230-449	5.6(12)		835±150	2	1.5
O + $CH_3CF=CH_2$ → products							
Oxygen atom + 1-Propene, 2-fluoro-							
69 MOS/JEN	RL	296	0.46			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Butene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.0(12) (73 HER/HUI). Current update (86 CVE) k=1.15(11)							
73 HER/HUI	SE	307	2.6(11)			2	1.3
86 CVE	RN	296	1.15(12)			2	
Derived from relative k (69 MOS/JEN) using for 1-Butene k=2.50(12).							
Recommended value of k	RE	298	1.2(12)			2	1.2

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_2FCH=CH_2$ → products							
Oxygen atom + 1-Propene, 3-fluoro-							
69 MOS/JEN	RL	296	0.21			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Propene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=4.4(11) (73 HER/HUI). Current update (86 CVE) k=5.1(11)							
73 HER/HUI	SE	296	5.1(11)			2	1.4
86 CVE	RN	296	5.0(11)			2	
Derived from relative k (69 MOS/JEN) using for 1-Propene k=2.4(12).							
Recommended value of k	RE	298	5.0(11)			2	1.2
O + $CH_3CH=CF_2$ → products							
Oxygen atom + 1-Propene, 1,1-difluoro-							
69 MOS/JEN	RL	296	0.45			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Propene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=9.5(11) (73 HER/HUI). Current update (86 CVE) k=1.1(12)							
73 HER/HUI	SE	296	1.1(12)			2	1.4
86 CVE	RN	296	1.08(12)			2	
Derived from relative k (69 MOS/JEN) using for 1-Propene k=2.4(12).							
Recommended value of k	RE	298	1.1(12)			2	1.2
O + $CF_3CH=CH_2$ → products							
Oxygen atom + 1-Propene, 3,3,3-trifluoro-							
69 MOS/JEN	RL	296	0.057			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.3(10) (73 HER/HUI). Current update (86 CVE) k=2.6(10)							
73 HER/HUI	SE	296	2.6(10)			2	1.4
86 CVE	RN	296	2.51(10)			2	
Derived from relative k (69 MOS/JEN) using for $CH_2=CH_2$ k=4.40(11).							
Recommended value of k	RE	298	2.5(10)			2	1.2

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CF_3CF=CF_2$ → products							
Oxygen atom + 1-Propene, 1,1,2,3,3,3,-hexafluoro- (perfluoropropylene)							
65 SAU/HEI2	RL	297	0.034			2/2	
k/k_{ref} from products in competing expts. Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.7(10) (73 HER/HUI). For updated normalized k see 86 CVE.							
66 SAU/HEI	RL	297-398	*)		*)	2/2	
*) k/k_{ref} from products in competing expts.: 0.0357(297K), 0.0385(343K), 0.0488(398K) Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normd. k(298)=1.7(10) (73 HER/HUI); updates: k(298)=1.57(10), A=7.81(11), B=1166 (86 CVE).							
86 CVE	RN	297	1.52(10)			2	
Derived from relative k (65 SAU/HEI2) using for $CH_2=CH_2$ k=4.40(11).							
	RN	298	1.57(10)			2	
Derived from relative k (66 SAU/HEI) using for $CH_2=CH_2$ k=4.40(11).							
	RN	297-398	7.81(11)		1166	2	
Derived from relative k's (66 SAU/HEI) using for $CH_2=CH_2$ A=6.40(12), B=800.							
Recommended value of k	RE	298	1.5(10)			2	1.2
Recommended values of Arrhenius A and B	RE	297-398	7.8(11)		1166±200	2	1.5
O + $CF_2=CFCF=CF_2$ → products							
Oxygen atom + 1,3-Butadiene, 1,1,2,3,4,4-hexafluoro- (1,3-Perfluorobutadiene)							
71 STO/HEI	RL	305	0.50			2/2	
k/k_{ref} from products in competing expts. Ref. Rn: O + $CH_2=CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.5(11) (73 HER/HUI). For updated normalized k see 86 CVE.							
73 HER/HUI	SE	305	2.5(11)			2	1.4
86 CVE	RN	305	2.20(11)			2	
Derived from relative k (71 STO/HEI) using for Ethylene k=4.40(11).							
Recommended value of k	RE	298	2.2(11)			2	1.2

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=$CHCH_2Cl$ → products							
Oxygen atom + 1-Propene, 3-chloro-							
84 PAR/SAW1	EX	299±4	(6.14±0.36)(11)			2	
Fast-flow reactor-Photoionization mass spec. Quoted error is 1σ; estimd. accuracy: ±20%. At P=0.6-3.5 torr, k is P invariant (±20%).							
Recommended value of k	RE	298	6.1(11)			2	1.2
O + $CH_3C(CF_3)$=CH_2 → products							
Oxygen atom + 1-Propene, 2-trifluoromethyl-							
68 MOS/JEN	RL	296	0.077			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Butene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.7(11) (73 HER/HUI). For updated normalized k see 86 CVE.							
71 MOS	RL	296	0.55			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.6(11) (73 HER/HUI). For updated normalized k see 86 CVE.							
73 HER/HUI	SE	296	2.0(11)			2	1.4
74 JON/MOS	RL	298-423	0.909		142	2/2	
k/k_{ref} from products in competing expts.: 298K: 0.552; 423K: 0.637. Ref. Rn: O + CH_2=CH_2 → products O from Hg-photosensitized decompn. of N_2O. Current normalized values (86 CVE): k(298)=2.43(11), A=5.82(12), B=942							
86 CVE	RN	296	1.93(11)			2	
Derived from relative k (68 MOS/JEN) using for 1-Butene k=2.50(12).							
	RN	296	2.42(11)			2	
Derived from relative k (71 MOS) using for Ethylene k=4.4(11).							
	RN	298	2.43(11)			2	
Derived from relative k (74 JON/MOS) using for Ethylene k=4.4(11).							
	RN	298-423	5.82(12)		942	2	
Derived from relative k's (74 JON/MOS) using for Ethylene A=6.40(12), B=800.							
Recommended value of k	RE	298	(2.26±0.29)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	200-450	5.8(12)		942±200	2	1.5

Table 4.2. **Data for O(^{3}P) Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_2FCH_2CH{=}CH_2$ → products							
Oxygen atom + 1-Butene, 4-fluoro-							
69 MOS/JEN	RL	296	0.575			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Butene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.3(12) (73 HER/HUI). Current update: k=1.44(12) (86 CVE)							
73 HER/HUI	SE	296	1.5(12)			2	1.4
86 CVE	RN	296	1.44(12)			2	
Derived from relative k (69 MOS/JEN) using for 1-Butene k=2.50(12).							
Recommended value of k	RE	298	1.4(12)			2	1.2
O + $CH_3CH_2CF{=}CF_2$ → products							
Oxygen atom + 1-Butene, 1,1,2-trifluoro-							
69 MOS/JEN	RL	296	1.00			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + 1-Propene → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=2.1(12) (73 HER/HUI). Current update: k=2.4(12) (86 CVE)							
69 MOS/JEN	RL	296	11.0			2/2	
k/k_{ref} from products in competing expts.: Ref. Rn: O + $CH_3C(CF_3){=}CH_2$ → products O from Hg-photosensitized decompn. of N_2O. Normalized absolute k=1.9(12) (73 HER/HUI). Current update: k=2.49(12) (86 CVE)							
73 HER/HUI	SE	296	2.0(12)			2	1.4
86 CVE	RN	296	2.4(12)			2	
Derived from relative k (69 MOS/JEN) using for 1-Propene k=2.4(12).							
	RN	296	2.49(12)			2	
Derived from relative k (69 MOS/JEN) using for $CH_3C(CF_3){=}CH_2$ k=2.26(11).							
Recommended value of k	RE	298	(2.45±0.05)(12)			2	1.2
O + $CH_2{=}CO$ → adduct(EXV)							
Oxygen atom + Ethenone (Ketene)							
Initial adduct → HC(O)C(O)H(EXV) → 2HCO (mainly): (see 74 MAC/THR)							
68 CAR/GAY	EX	298	5.30(11)			2	
Discharge flow. Time of flight mass spec.							

Table 4.2. Data for $O(^3P)$ Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CO → adduct(EXV) -- Continued							
73 JON/BAY	EX	296±2	(1.7±0.4)(11)			2	
Flow system with 0.5-4 torr N_2 as principal flow gas. Photoionizn. mass spec. analysis. O atoms from N + NO → N_2 + O							
74 MAC/THR	EX	293	(3.4±0.3)(11)			2	
Discharge flow system-ESR spectroscopy. or O+NO chemiluminescence. Quoted error is one standard deviation.							
83 WAS/HAT	EX	298	(2.59±2.41)(11)			2	
Discharge flow-photoionization mass spectr.	EX	230-449	(1.76±0.47)(12)		679±76	2	
Pulse radiolysis-Resonance absorption. k(298K)=1.80(11) (calcd. from Arrh. Eq.) k(296K)=(1.90±0.28)(11) (measured)							
Recommended value of k	RE	298	(2.37±0.79)(11)			2	1.2
Recommended values of Arrhenius A and B	RE	230-449	1.8(12)		680±200	2	1.5
O + CH_3CH=CO → adduct(EXV)							
Oxygen atom + 1-Propen-1-one							
83 WAS/HAT	EX	298	(6.99±0.78)(12)			2	
Discharge flow-photoionization mass spectr.	EX	230-449	(2.89±0.79)(12)		-249±82	2	
Pulse radiolysis-Resonance absorption. k(298K)=6.65(12) (calcd. from Arrh. Eq.) k(296K)=(6.26±1.02)(12) (measured)							
Recommended value of k	RE	298	(6.8±0.2)(12)			2	1.2
Recommended values of Arrhenius A and B	RE	230-449	2.9(12)		-250±100	2	1.5
O + CH_3CH_2CH=CO → adduct(EXV)							
Oxygen atom + 1-Buten-1-one							
83 WAS/HAT	EX	298	(8.19±0.66)(12)			2	
Discharge flow-photoionization mass spectr.	EX	230-449	(3.23±0.50)(12)		-224±47	2	
Pulse radiolysis-Resonance absorption. k(298K)=6.84(12) (calcd. from Arrh. Eq.) k(296K)=(6.50±1.33)(12) (measured)							
Recommended value of k	RE	298	(7.34±0.84)(12)			2	1.2
Recommended values of Arrhenius A and B	RE	230-449	3.2(12)		-220±100	2	1.5

Table 4.2. **Data for O(^{3}P) Reactions with Haloalkenes and Ketenes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $(CH_3)_2C{=}CO$ → adduct(EXV)							
Oxygen atom + 1-Propen-1-one, 2-methyl-							
83 WAS/HAT	EX	298	(3.64±0.39)(13)			2	
Discharge flow-photoionization mass spectr.							
	EX	296	(2.42±0.28)(13)			2	
	EX	230-449	(3.57±0.57)(12)		-569±43	2	
Pulse radiolysis-Resonance absorption.							
k(298K)=2.40(13) (calcd. from Arrh. Eq.)							
Recommended value of k	RE	298	(3.0±0.6)(13)			2	1.2
Recommended values of Arrhenius A and B	RE	230-449	3.6(12)		-570±100	2	1.5

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH≡CH → products							
Oxygen atom + Ethyne (Acetylene)							
Main rn. products are: $CO + CH_2$ and H + .CHCO							
65 ARR/BRE1	EX	*)	1.2(11)		*)		2
A brief announcement in a Comment.							
Discharge flow. Time-of-flight mass spec.							
*)Temp. probably close to 298K. P=1-2 torr.							
E(Arrhs.) less than 1 kcal/mol (B<500).							
65 ARR/BRE2	EX	*)	(5.4±1.7)(10)		*)		2
Moderately fast flow system. Time-of-flight							
mass spectrometer and photometry.							
*)"Room temperature" (probably approx. 298K).							
E(Arrhs.) less than 1 kcal/mol (B<500).							
65 SUL/WAR	EX	*)	(9.0±1.8)(10)				2
*)Temp. probably close to 298K.							
Discharge fast flow. Mass spectrometer.							
65 AVR/KOL	EX	393-563	1.75(11)		1560		2
k(298K)=9.3(8) (extrapoln. of Arrhs. Eq.).							
O from high-voltage discharge in O_2.							
k derived from rates of product formation.							
66 SAU/HEI	RL	297-398	*)		1310		2/2
*) k/k_{ref} from products in competing expts:							
0.193(297K), 0.296(343K), 0.566(398K)							
Ref. Rn: O + CF_2=CF_2 → products							
O from Hg-photosensitized decompn. of N_2O.							
Normalized k(297K)=1.0(11) (73 HER/HUI).							
Current update: k(297K)=1.1(11).							
67 NIK	EX	300	(1.1±0.2)(11)				2
Fast flow system-Time of flight mass spec.							
O from N+NO rn.							
67 BRO/THR	EX	298	(9.2±0.4)(10)				2
Fast-flow reactor. ESR. N_2 carrier gas.							
O from N+NO Rn. Total P about 2 torr.							
69 HOY/WAG	EX	243-673	1.2(13)		1510		2
k(298K)=7.6(10) (calcd. from Arrh. Eq.).							
Flow system with continuous ESR and mass							
spec. analysis. k derived from O-decays.							
69 WES/DEH1	EX	298	(8.9±0.3)(10)				2
	EX	230-450	2.0(13)		1610		2
Curved Arrhenius plot for T=195-616K. It is							
approx. linear for T=230-450K, where							
k(298K)=9.0(10) (calcd. from Arrh. Eq.).							
Fast-flow reactor with ESR detection.							
O by microwave discharge of trace O_2 in He.							

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH≡CH → products -- Continued							
69 BRA/TSE Discharge flow. ESR. O from N+NO Rn.	EX	298	(1.1±0.1)(11)			2	
69 JAM/GLA Fast flow system-CH* chemiluminescence. k(298K)=7.01(10) (calcd. from Arrh. Eq.).	EX	273-729	(1.43±0.50)(13)		1585±100	2	
71 STU/NIK *) Uncertainty limits given as +5%,-10%. O by vacuum uv flash photolysis of NO, monitored by O+NO chemiluminescence.	EX	300	(7.89± *))(10)			2	
73 PEE/MAH k(298K)=1.0(11) (calcd. from Arrh. Eq.). Composition profiles of unidimensional ethylene flames obtained by molecular beam sampling and mass spectr. analysis. k derived from the mole flux gradients.	EX	1200-1700	5.2(13)		1862	2	
73 JON/BAY Flow system with 0.5-4 torr N_2 as principal flow gas. Photoionizn. mass spec. analysis. O atoms from N + NO → N_2 + O	EX	296±2	(9.7±1.5)(10)			2	
73 HER/HUI	SE	298	9.5(10)			2	1.1
	SE	1000	8.3(12)			2	1.4
	SE	200-700	1.4(13)		1500	2	1.2
77 VAN/VAN Study of CH≡CH/O_2 flame front structure. Molecular beam sampling coupled with mass spectrometer. k(298K)=7.8(10) (calcd. from Arrh. Eq.).	EX	700-1430	6.7(13)		2013	2	
77 WES/DEH Flash photolysis. Resonance fluorescence. k from [O] decay. (k from the decay of the chemiluminescent background is (8.2±0.2)(10)).	EX	297±1	(7.2±0.2)(10)			2	
81 WEL k(298K)=8.7(10) (calcd. from Arrh. Eq.). Discharge flow system. Mass spec. analysis.	EX	295-1333	1.1(13)		1443	2	
83 HOM/WEL k(298K)=8.8(10) (calcd. from Arrh. Eq.). High temp. low pressure discharge flow. Nozzle beam sampling-Quadrupole mass spec. P=2 torr. O from N + NO → N_2 + O Rn.	EX	300-1300	(1.6±0.5)(13)		1550±70	2	
Recommended value of k	RE	298	9.0(10)			2	1.2
Recommended values of Arrhenius A and B Provisional recommendations.	RE	250-1300	1.6(13)		1550±100	2	1.5

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH≡CH → CO + CH_2							
A path in the Rn. O + CH≡CH → products							
For "branching ratios" see 86 PEE/SCH and							
references quoted in 86 PEE/SCH.							
81 ALE/ARU	EX	298-608	(1.8±0.18)(13)		1625±110	2	
k(298K)=7.7(10) (calcd. from Arrh. Eq.).							
Monitored (by resonance-fluorescence)							
[O] and [H] under jet conditions.							
81 LOH/ROT	EX	1500-2570	1.2(14)		3300	2	
(Long extrapoln. of Arrh. Eq.: k(298)=1.9(9))							
Shock tube. Atomic resonance absorption							
spectroscopy (ARAS). (See also 82 ROT/LOH).							
82 ROT/LOH	EX	1500-2600	1.2(14)		3300	2	
Data first reported in 81 LOH/ROT.							
O + CH≡CH Rn. behind reflected shock-waves in							
Ar. O from fast N_2O decomposition. Atomic Re-							
sonance Absorption Spectroscopy (ARAS).							
84 WAR	SE	300-2500	2.1(12)	1.5	850	2	2
Recommended values of Arrhenius A and B	RE	300-2500	2.1(12)	1.5	850	2	2
O + CH≡CH → H + CH=C=O							
A path in the Rn. O + CH≡CH → products							
For "branching ratios" see 86 PEE/SCH and							
references quoted in 86 PEE/SCH.							
81 ALE/ARU	EX	298-608	(9.0±2.4)(12)		2285±220	2	
k(298K)=4.2(9) (calcd. from Arrh. Eq.).							
Monitored (by resonance-fluorescence)							
[O] and [H] under jet conditions.							
81 LOH/ROT	EX	1500-2570	4.3(14)		6100	2	
(Long extrapoln. of Arrh. Eq.: k(298)=5.5(5))							
Shock tube. Atomic resonance absorption							
spectroscopy (ARAS). (See also 82 ROT/LOH).							
82 ROT/LOH	EX	1500-2600	4.3(14)		6100	2	
Data first reported in 81 LOH/ROT.							
Reaction of O atoms with CH≡CH behind							
reflected shock-waves, in Ar diluent.							
O atoms generated by fast N_2O de-							
composition. Atomic-resonance-absorp-							
tion-spectrometry (ARAS).							
84 WAR	SE	1000-2500	4.3(14)	0	6100	2	3
Recommended values of Arrhenius A and B	RE	300-600	9.0(12)		2300±300	2	1.5
k(298K)=4.0(9) (calcd. from Arrh. Eq.).							
Recommended values of Arrhenius A and B	RE	1000-2500	4.3(14)		6100	2	3

Table 4.3. **Data for $O(^3P)$ Reactions with Alkynes** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CD≡CD → products							
Oxygen atom + Ethyne-d2 (Dideuteroacetylene)							
71 STU/NIK	EX	300	(7.89± *))(10)			2	
*) Uncertainty limits given as +5%,-10%. O by vacuum uv flash photolysis of NO, monitored by O+NO chemiluminescence.							
Recommended value of k	RE	298	8.6(10)			2	1.2
O + $CH_3C{\equiv}CH$ → products							
Oxygen atom + 1-Propyne (Methylacetylene)							
Main reaction channel at lower T is:							
O + $CH_3C{\equiv}CH$ → CO + CH_3CH:							
67 BRO/THR	EX	298	(4±1)(11)			2	
Fast-flow reactor. ESR. N_2 carrier gas. O from N+NO Rn. Total P about 2 torr.							
73 HER/HUI	SE	298	4(11)			2	2
74 HER/WAG	EX	298	4.4(11)			2	
	EX	290-360	1.3(13)		1007±200	2	
k(298K)=4.4(11) (calcd. from Arrh. Eq.). Isothermal flow system. P=5 torr. Carrier gas He. O from microwave discharge in O_2 or NO, monitored by time-of-flight mass spectromtr.							
75 ARR/COX	EX	298-600	(1.39±0.36)(13)		981±352	2	
k(298K)=5.2(11) (calcd. from Arrh. Eq.). Discharge-flow system. O from N+NO rn., monitored by chemiluminescence. Total P= 1-3 torr. Estimated 25% uncertainty in k.							
81 WEL	EX	295-1333	1.5(13)		1058	2	
k(298K)=4.3(11) (calcd. from Arrh. Eq.). Discharge flow system. Mass spec. analysis. See also 83 HOM/WEL.							
81 ALE/DUB	EX	295-545	(8.4±2.4)(12)		866±110	2	
k(295K)=4.6(11) (calcd. from Arrh. Eq.). Monitored (by resonance-fluorescence) [O] and [H] under jet conditions.							
83 HOM/WEL	EX	300-1300	(1.5±0.4)(13)		1060±140	2	
k(298K)=4.3(11) (calcd. from Arrh. Eq.). High temp. low pressure discharge flow. Nozzle beam sampling-Quadrupole mass spec. P=2 torr. O from N + NO → N_2 + O Rn.							
84 WAR	SE	300-2000	1.5(13)		1058	2	
k(298K)=4.3 (11) (calcd. from Arrh. Eq.).							
Recommended value of k	RE	298	(4.47±0.41)(11)			2	1.1
Recommended values of Arrhenius A and B	RE	290-1300	1.31(13)		1000±100	2	1.2

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_3C{\equiv}CH \rightarrow H + [C_3H_3O]^{\cdot}$							
A path in the Rn. $O + CH_3C{\equiv}CH \rightarrow$ products							
81 ALE/DUB	EX	295-545	(3.6±1.2)(12)		1320±220	2	
Monitored O and H atoms under jet conditions. Resonance-fluorescence. Arrhs. Eqn. gives upper limit of k, eg. k(298K) ≤ 4.3(10) (calcd. from Arrh. Eq.).							
Recommended upper limit value of k	RE	298	≤ 4.3(10)			2	1.2
Provisional recommendation.							
Recommended values of Arrhenius A and B defining upper limit of k. Provisional recommendations.	RE	295-545	3.6(12)		1320±400	2	1.5
$O + CH{\equiv}CC{\equiv}CH \rightarrow$ products							
Oxygen atom + 1,3-Butadiyne (Diacetylene)							
66 NIK/WEI	EX	300	(3.98±0.48)(11)			2	
Discharge-flow system. Mass spectrometer.							
67 NIK	EX	300	(9.0±1.2)(11)			2	
Fast flow system-Time of flight mass spectr. O from N+NO rn.							
73 JON/BAY	EX	296±2	(1.6±0.5)(12)			2	
Flow system with 0.5-4 torr N_2 as principal flow gas. Photoionizn. mass spec. analysis. O atoms from $N + NO \rightarrow N_2 + O$ Rn.							
73 HER/HUI	SE	300	9(11)			2	1.4
75 HOM/SCH	EX	297-343	8.0(13)		1230	2	
k(298K)=1.3(12) (calcd. from Arrh. Eq.). Isothermal low pressure flow system. Quadrupole mass spectrometer. O from microwave discharge in O_2/He mixtures or from N+NO rn.							
81 WEL	EX	295-1000	2.7(13)		866	2	
k(298K)=1.5(12) (calcd. from Arrh. Eq.). Discharge flow system. Mass spec. analysis.							
83 HOM/WEL	EX	300-1300	(2.8±0.6)(13)		870±80	2	
k(298K)=1.5(12) (calcd. from Arrh. Eq.). High temp. low pressure discharge flow. Nozzle beam sampling-Quadrupole mass spec. P=2 torr. O from $N + NO \rightarrow N_2 + O$ Rn.							
84 WAR	SE	300-1000	2.7(13)		866	2	
k(298K)=1.5(12) (calcd. from Arrh. Eq.).							
Recommended value of k	RE	298	1.4(12)			2	1.2
Recommended values of Arrhenius A and B	RE	298-1300	4.5(13)		990±300	2	1.2

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH_2=CHC≡CH → products							
Oxygen atom + 1-Butene-3-yne (Vinylacetylene)							
83 HOM/WEL	EX	300-1300	(3.0±1.1)(13)		910±100	2	
k(298K)=1.4(12) (calcd. from Arrh. Eq.). High temp. low pressure discharge flow. Nozzle beam sampling-Quadrupole mass spec. P=2 torr. O from N + NO → N_2 + O Rn.							
Recommended value of k	RE	298	1.4(12)			2	1.2
Recommended values of Arrhenius A and B	RE	298-1300	3.0(13)		910±200	2	1.5
O + CH_3CH_2C≡CH → CO + CH_3CH=CH_2							
Oxygen atom + 1-Butyne (Ethylacetylene)							
75 HER/WAG1	EX	290-357	1.7(13)		800	2	
k(298K)=1.2(12) (calcd. from Arrh. Eq.). Isothermal flow system. P=5 torr. Carrier gas He. O from microwave discharge in O_2 or NO, monitored by time-of-flight mass spectromtr.							
77 UMS/LIN	RN	298	5.0(11)			2	
NO_2 Flash-photolysis-CO laser resonan. absorption. Ref. rn.: O+propyne → products. k/k(ref) from computer modeling of CO formn. rates, normalized by taking k(ref)=4.2(11).							
83 HOM/WEL	EX	300-1300	(2.3±0.7)(13)		870±80	2	
k(298K)=1.2(12) (calcd. from Arrh. Eq.). High temp. low pressure discharge flow. Nozzle beam sampling-Quadrupole mass spec. P=2 torr. O from N + NO → N_2 + O Rn.							
Recommended value of k	RE	298	1.2(12)			2	1.2
Recommended values of Arrhenius A and B	RE	298-1300	2.0(13)		835±100	2	1.5
O + CH_3C≡CCH_3 → CO + CH_3CH=CH_2							
Oxygen atom + 2-Butyne (Dimethylacetylene)							
75 HER/WAG2	EX	298	2.9(12)			2	
	EX	290-360	6(13)		900	2	
Estimated error limits approx. ±25%. Isothermal flow system. P=5 torr. Carrier gas He. O from microwave discharge in O_2 or NO, monitored by time-of-flight mass spectromtr.							

Table 4.3. Data for $O(^3P)$ Reactions with Alkynes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_3C{\equiv}CCH_3 \rightarrow CO + CH_3CH{=}CH_2$ -- Continued							
77 UMS/LIN NO_2 Flash-photolysis-CO laser resonant absorption. Ref. rn.: O+propyne → products. k/k(ref) from computer modeling of CO formn. rates, normalized by taking k(ref)=4.2(11).	RN	298	1.6(12)			2	
Recommended value of k (chosen the more direct 75 HER/WAG2 value)	RE	298	2.9(12)			2	1.2
Recommended values of Arrhenius A and B (chosen the more direct 75 HER/WAG2 values)	RE	290-360	6(13)		900±300	2	1.5
$O + CH_3CH_2CH_2C{\equiv}CH \rightarrow CO(EXV) + CH_3CH_2CH_2CH$:							
Oxygen atom + 1-Pentyne (n-Propylacetylene)							
80 SHA/BUR NO_2 Flash-photolysis-CO laser resonant absorption. Ref. rn.: O + CH≡CH → products. k/k(ref) from computer modeling of CO formn. rates, normalized by taking k(ref)=9.4(10).	RN	300	(4.9±0.6)(11)			2	
Recommended value of k (80 SHA/BUR value using k(ref)=8.6(10)). Provisional recommendation.	RE	298	4.5(11)			2	1.5
$O + CH_3CH_2CH_2CH_2C{\equiv}CH \rightarrow CO(EXV)$ $+ CH_3CH_2CH_2CH_2CH$:							
Oxygen atom + 1-Hexyne (n-Butylacetylene)							
80 SHA/BUR NO_2 Flash-photolysis-CO laser resonant absorption. Ref. rn.: O + CH≡CH → products. k/k(ref) from computer modeling of CO formn. rates, normalized by taking k(ref)=9.4(10).	RN	300	(3.6±0.4)(11)			2	
Recommended value of k (80 SHA/BUR value using k(ref)=8.6(10)). Provisional recommendation.	RE	298	3.3(11)			2	1.5

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + C_6H_6 \rightarrow$ products							
Oxygen atom + Benzene							
61 BOO/CVE	RL	393-494	1.04		1993	2/2	
k/k_{ref} from products in competing expts.: 393K: 6.55(-3); 494K: 1.84(-2). k_{ref}: O + Cyclopentene → products Normalized A=1.49(13), B=2033 (86 CVE)							
68 MAN/SAU	EX	*)	(3.6±0.7)(10)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
72 BON/KIM	EX	255-305	(3.8±1.5)(13)		2214±252	2	
Discharge fast flow (O_2 in He)-Mass spectrometer. k(298K): (2.8±0.70)(10). (Same k's obtained using O from N+NO rn.)							
73 HER/HUI	SE	298	2.4(10)			2	2
	SE	250-500	2.0(13)		2000	2	2
74 ATK/PIT2	EX	300	(1.44±0.2)(10)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	1.11(13)		2003±200	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
75 COL/SIN	EX	298-462	(1.09±0.64)(13)		2115±216	2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are 95% confidence limits. k(298K)=(9.3±0.5)(9) (calcd. from Arrhs. Eq.)							
79 ATK/PIT	EX	298	(1.20±0.12)(10)			2	
	EX	299-440	1.01(13)		2011±100	2	
Flash photolysis-O+NO chemiluminescence. O from vacuum uv photolysis of O_2 and NO. Quoted errors are estimated overall limits.							
82 NIC/GUM1	EX	298	(9.52±2.35)(9)			2	
	EX	298-867	(2.78±0.41)(13)		2470±80	2	
Flash photolysis-Resonance fluorescence. O from vacuum uv photolysis of O_2. Quoted errors are 2 standard deviations.							
86 CVE	RN	393-494	1.49(13)		2033	2	
Derived from relative k data (61 BOO/CVE) using for Cyclopentene A=1.43(13), B=40. k(298K)=1.62(10) (calcd. from Arrhs. Eq.)							
Recommended value of k	RE	298	(1.22±0.29)(10)			2	1.3
Recommended values of Arrhenius A and B	RE	298-600	1.52(13)		2130±200	2	2

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + C_6D_6 → products							
Oxygen atom + Benzene-d6							
72 BON/KIM	RL	298	1.03±0.02			2/2	
Ref. Rn.: O + C_6H_6 → products							
k/k_{ref}: from ratio of the benzenes used.							
82 NIC/GUM1	EX	376-944	(2.65±0.66)(13)		2450±130	2	
Flash photolysis-Resonance fluorescence.							
O from vacuum uv photolysis of O_2.							
Quoted errors are 2 standard deviations.							
k(298K)=7.12(9) (calcd. from Arrhs. Eq.)							
Recommended value of k	RE	298	*)			2	1.3
Recommended values of Arrhenius A and B	RE	376-944	*)		*)	2	2
*) Same as for O + C_6H_6							
O + $C_6H_5CH_3$ → products							
Oxygen atom + Benzene, methyl-							
61 JON/CVE	RL	393-495	1.02		1600	2/2	
k/k_{ref} from products in competing expts.							
393.4K: 1.74(-2); 495.3K: 4.02(-2).							
k_{ref}: O + Cyclopentene → products							
Normalized A=1.45(13), B=1640 (86 CVE)							
68 MAN/SAU	EX	*)	(1.4±0.3)(11)			2	
*)T probably ~298K. O from pulse radiolysis							
of CO_2 or N_2O. k from absorption tracings							
of (not positively identified) transients.							
70 GRO/MOS	RL	303	4.37			2/2	
k/k_{ref}: from ratio of the phenols formed.							
Ref. Rn.: O + Benzene → products							
(Tar formed in the reaction assumed not							
to affect phenol ratios).							
Normalized k(298)=5.33(10) (86 CVE)							
73 HER/HUI	SE	298	1.4(11)			2	2
74 ATK/PIT2	EX	300	(4.50±0.45)(10)			2	
Phase shift-O+NO chemiluminescence.							
O from Hg-photosensitized decomp. of N_2O.							
Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	8.2(12)		1560±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + C_6H_5CH_3 \rightarrow$ products -- Continued							
75 COL/SIN	EX	298-462	(2.30±0.11)(13)		1940±20	2	
Phase shift-O+NO chemiluminescence.							
O from Hg-photosensitized decomp. of N_2O.							
Quoted errors are 95% confidence limits.							
k(298K)=(3.4±0.2)(10) (calcd. from Arrhs. Eq.)							
75 FUR/EBA	EX	373-510	(5.24±1.47)(12)		1350±100	2	
Microwave discharge-fast-flow reactor. GLC.							
O from N+NO Rn. Quoted error=1σ.							
k(298K)=5.64(10) (calcd. from Arrh. Eq.)							
79 ATK/PIT	EX	298	(5.79±0.58)(10)			2	
	EX	299-440	9.88(12)		1535±100	2	
Flash photolysis-O+NO chemiluminescence.							
O from vacuum uv photolysis of O_2 and NO.							
Quoted errors are estimated overall limits.							
82 NIC/GUM1	EX	298	(4.30±0.54)(10)			2	
	EX	298-932	(2.57±0.35)(13)		1910±70	2	
Flash photolysis-Resonance fluorescence.							
O from vac. uv photol. of O_2. Error=2σ.							
86 CVE	RN	393-495	1.45(13)		1640	2	
Derived from relative k data (61 JON/CVE)							
using for Cyclopentene A=1.43(13), B=40.							
k(298K)=5.90(10) (calcd. from Arrhs. Eq.)							
	RN	303	5.33(10)			2	
Derived from relative k data (70 GRO/MOS)							
using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	5.0(10)			2	1.4
Recommended values of Arrhenius A and B	RE	298-932	1.63(13)		1720±200	2	2
$O + C_6H_5CD_3 \rightarrow$ products							
Oxygen atom + 1,1,1-trideuterotoluene							
82 NIC/GUM1	EX	298	(5.18±0.56)(10)			2	
	EX	298-944	(2.23±0.46)(13)		1880±100	2	
Flash photolysis-Resonance fluorescence.							
O from vac. uv photol. of O_2. Error=2σ.							
Recommended value of k	RE	298	5.2(10)			2	1.5
Recommended values of Arrhenius A and B	RE	298-944	2.2(13)		1800±200	2	2

Table 4.4. **Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons** -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $C_6H_5CH_2CH_3$ → products							
Oxygen atom + Benzene, ethyl-							
68 MAN/SAU	EX	*)	(3.2±0.8)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	4.95			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios). Normalized k(298)=6.03(10) (86 CVE)							
73 HER/HUI	SE	298	3.2(11)			2	2
86 CVE	RN	303	6.03(10)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	6(10)			2	2
O + o-$CH_3C_6H_4CH_3$ → products							
Oxygen atom + o-Xylene							
68 MAN/SAU	EX	*)	(6.7±1.6)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	10.0			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios). Normalized k(298)=1.22(11) (86 CVE)							
73 HER/HUI	SE	298	6.7(10)			2	2
74 ATK/PIT2	EX	299	(1.05±0.11)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	6.25(12)		1223±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
82 NIC/GUM2	EX	298	(1.33±0.12)(11)			2	
	EX	298-600	(2.35±0.51)(13)		1540±80	2	
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O_2. Error=2σ.							

Table 4.4. Data for O(^{3}P) Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + o-$CH_3C_6H_4CH_3$ → products -- Continued							
86 CVE	RN	303	1.22(11)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	1.2(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-600	(1.5±1.2)(13)		1382±300	2	2
O + o-$CD_3C_6D_4CD_3$ → products							
Oxygen atom + o-Xylene-d10							
82 NIC/GUM2	EX	298	(1.20±0.13)(11)			2	
	EX	298-600	(2.06±0.37)(13)		1550±70	2	
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O_2. Error=2σ.							
Recommended value of k	RE	298	1.2(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-600	2.1(13)		1550	2	2
O + m-$CH_3C_6H_4CH_3$ → products							
Oxygen atom + m-Xylene							
68 MAN/SAU	EX	*)	(7.7±2.0)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	23.0			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios). Normalized k(298)=2.81(11) (86 CVE)							
73 HER/HUI	SE	298	7.7(11)			2	2
74 ATK/PIT2	EX	299	(2.12±0.21)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	7.7(12)		1082±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
82 NIC/GUM2	EX	298	(2.37±0.26)(11)			2	
	EX	298-600	(2.28±0.51)(13)		1350±90	2	
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O_2. Error=2σ.							
86 CVE	RN	303	2.81(11)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + m-$CH_3C_6H_4CH_3$ → products -- Continued							
Recommended value of k	RE	298	2.4(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-600	(1.5±1.1)(13)		1216±200	2	2
O + m-$CD_3C_6D_4CD_3$ → products							
Oxygen atom + m-Xylene-d10							
82 NIC/GUM2	EX	298	(2.40±0.24)(11)			2	
	EX	298-600	(1.67±0.36)(13)		1290±80	2	
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O_2. Error=2σ. k(298K)=2.20(11) (calcd. from Arrh. Eq.)							
Recommended value of k	RE	298	2.4(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-600	(1.7±0.4)(13)		1290±80	2	2
O + p-$CH_3C_6H_4CH_3$ → products							
Oxygen atom + p-Xylene							
68 MAN/SAU	EX	*)	(4.5±1.4)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	9.77			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products Normalized k(298)=1.19(11) (86 CVE)							
73 HER/HUI	SE	298	4.5(11)			2	2
74 ATK/PIT2	EX	300	(1.09±0.11)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	7.9(12)		1278±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
82 NIC/GUM2	EX	298	(1.32±0.13)(11)			2	
	EX	298-600	(2.35±0.46)(13)		1540±90	2	
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O_2. Error=2σ.							
86 CVE	RN	303	1.19(11)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	1.2(11)			2	1.2
Recommended values of Arrhenius A and B	RE	298-600	(1.57±1.10)(13)		1409±185	2	2

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err factor
O + $C_6H_5C(CH_3)_3$ → products							
Oxygen atom + Benzene, t-butyl-							
70 GRO/MOS	RL	303	3.60			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios).							
86 CVE	RN	303	4.39(10)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	4(10)			2	2
Provisional recommendation.							
O + 1,2,3-$(CH_3)_3C_6H_3$ → products							
Oxygen atom + Benzene, 1,2,3-trimethyl-							
70 GRO/MOS	RL	303	25.0			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios).							
74 ATK/PIT2	EX	300	(6.9±0.7)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	1.03(13)		805±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
86 CVE	RN	303	3.05(11)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	6.9(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-400	1.0(13)		800±300	2	2
O + 1,2,4-$(CH_3)_3C_6H_3$ → products							
Oxygen atom + Benzene, 1,2,4-trimethyl-							
74 ATK/PIT2	EX	300	(6.0±0.6)(11)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	9.35(12)		830±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
Recommended value of k	RE	298	6(11)			2	1.3
Recommended values of Arrhenius A and B	RE	298-400	9(12)		800±300	2	2

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + 1,3,5-$(CH_3)_3C_6H_3$ → products							
Oxygen atom + Benzene, 1,3,5-trimethyl-							
70 GRO/MOS	RL	303	80.0			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios). Normalized k(298)=9.76(11) (86 CVE)							
74 ATK/PIT2	EX	300	(1.68±0.20)(12)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N_2O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	6.05(12)		388±150	2	
(See Notes in preceding entry, 74 ATK/PIT2)							
86 CVE	RN	303	9.76(11)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	1.6(12)			2	2
Recommended values of Arrhenius A and B	RE	298-600	6.0(12)		400±200	2	2
O + C_5H_5N → products							
Oxygen atom + Pyridine							
68 MAN/SAU	EX	*)	(1.0±0.3)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
73 HER/HUI	SE	298	1.0(11)			2	2
83 TAB/GON	EX	323-473	(2.9±0.3)(12)		1258±150	2	
Modulated microwave discharge (in Ar/N_2O) fast flow system. O+NO chemiluminescence. k(298K)=4.26(10) (calcd. from Arrh. Eq.)							
Recommended value of k	RE	298	4.3(10)			2	2
Provisional recommendation.							
Recommended values of Arrhenius A and B	RE	300-500	2.9(12)		1260±300	2	2
Provisional recommendation.							

Table 4.4. Data for $O(^3P)$ Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + C_6H_5Cl → products							
Oxygen atom + Benzene, chloro-							
68 MAN/SAU	EX	*)	(3.1±0.8)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
Recommended value of k	RE	298	3(11)			2	3
Provisional recommendation.							
O + C_6H_5F → products							
Oxygen atom + Benzene, fluoro-							
68 MAN/SAU	EX	*)	(2.7±0.6)(10)			2	
*)T probably ~298K. O from pulse radiolysis of CO_2 or N_2O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	0.67			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios).							
86 CVE	RN	303	8.17(9)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	8(9)			2	3
Provisional recommendation.							
O + $C_6H_5CF_3$ → products							
Oxygen atom + Benzene, trifluoromethyl-							
70 GRO/MOS	RL	303	0.29			2/2	
k/k_{ref}: from ratio of the phenols formed. Ref. Rn.: O + Benzene → products (Tar formed in the reaction assumed not to affect phenol ratios).							
86 CVE	RN	303	3.53(9)			2	
Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).							
Recommended value of k	RE	298	3.5(9)			2	3
Provisional recommendation.							

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