

# Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(<sup>3</sup>P) with Unsaturated Hydrocarbons

Cite as: Journal of Physical and Chemical Reference Data 16, 261 (1987); <https://doi.org/10.1063/1.555783>  
Submitted: 18 September 1986 . Published Online: 15 October 2009

R. J. Cvetanović



View Online



Export Citation

## ARTICLES YOU MAY BE INTERESTED IN

[Rate Constants for the Reactions of Atomic Oxygen \(O <sup>3</sup>P\) with Organic Compounds in the Gas Phase](#)

Journal of Physical and Chemical Reference Data 2, 467 (1973); <https://doi.org/10.1063/1.3253125>

[Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O\(<sup>3</sup>P\) with Saturated Organic Compounds in the Gas Phase](#)

Journal of Physical and Chemical Reference Data 17, 967 (1988); <https://doi.org/10.1063/1.555810>

[Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O\(<sup>3</sup>P\) with Sulfur Containing Compounds](#)

Journal of Physical and Chemical Reference Data 17, 1377 (1988); <https://doi.org/10.1063/1.555811>

Where in the world is AIP Publishing?  
*Find out where we are exhibiting next*



# Evaluated chemical kinetic data for the reactions of atomic oxygen O(<sup>3</sup>P) with unsaturated hydrocarbons

R. J. Cvetanović

Chemical Kinetics Division, Center for Chemical Physics, National Bureau of Standards, Gaithersburg, MD 20899

Received September 18, 1986; revised manuscript received January 30, 1987

Chemical kinetic data for reactions of O(<sup>3</sup>P) 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(<sup>3</sup>P), 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(<sup>3</sup>P); pyridine; rate of reaction; recommended kinetic parameters; unsaturated hydrocarbons.

## Contents

1. Introduction .....	261	2. Summary of Symbols and Units .....	264
1.1. Overview .....	261	3. Index of Reactions and Summary of Recommended Rate Parameters .....	265
1.2. Reaction Mechanisms .....	262	4. Tables of Chemical Kinetic Data .....	271
1.3. Selection of Recommended Rate Parameters and Their Uncertainty Factors .....	263	4.1. Data for O( <sup>3</sup> P) Reactions with Alkenes .....	271
1.4. Organization .....	263	4.2. Data for O( <sup>3</sup> P) Reactions with Haloalkenes and Ketenes .....	292
1.5. Guide to Summary of Recommended Rate Parameters .....	263	4.3. Data for O( <sup>3</sup> P) Reactions with Alkynes .....	307
1.6. Guide to Chemical Kinetic Data Tables ..	263	4.4. Data for O( <sup>3</sup> P) Reactions with Aromatic Hydrocarbons .....	314
1.7. Acknowledgments .....	264	5. References to the Data Tables .....	323
1.8. References to the Introduction .....	264		

## 1. Introduction

### 1.1. Overview

The present evaluation of chemical kinetic data for the elementary reactions of O(<sup>3</sup>P) 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(<sup>3</sup>P) 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 model-

ing 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(<sup>3</sup>P) 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<sup>1-3</sup> in O(<sup>3</sup>P) reactions with alkenes. Well established kinetic behavior of O(<sup>3</sup>P) 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(<sup>3</sup>P) 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.

©1987 by the U. S. Secretary of Commerce on behalf of the United States. This copyright is assigned to the American Institute of Physics and the American Chemical Society.  
Reprints available from ACS; see Reprints List at back of issue.

## 1.2. Reaction Mechanisms

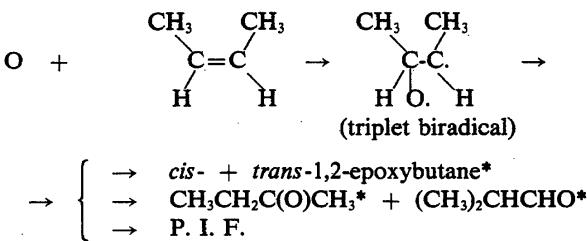
Interaction of a ground state oxygen atom,  $O(^3P)$ , with an unsaturated hydrocarbon molecule may in principle lead to any of the following three types of chemical change: 1) "abstraction" by the O atom of a H atom from the hydrocarbon, 2) "addition" of the O atom to the hydrocarbon, and 3) "replacement" 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<sup>4</sup>).

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<sup>2,5-7</sup> discuss the reaction mechanisms in considerable detail and provide lists of original references. The more recent review by Cvetanović and Singleton<sup>3</sup> 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.<sup>3</sup>

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<sup>3,8</sup>.

The general mechanism of O atom addition to alkynes<sup>7</sup> 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<sup>9</sup> 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<sup>10</sup>, 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.<sup>11</sup> In the present evaluation, the weighted least squares procedures were generally used to calculate the mean value and when an additive ( $\pm$ ) 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 ( $\pm$ ) deviations, are also approximate estimates.

The evaluation covers the investigated (and documented in the literature) O(<sup>3</sup>P) 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(<sup>3</sup>P) 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(<sup>3</sup>P) 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<sup>3</sup>mol<sup>-1</sup>s<sup>-1</sup> and their values are given in exponential form, written as (1.00±0.10)(11), which signifies (1.00±0.10)×10<sup>11</sup>. For recommended values of  $k$  and  $A$ , the additive ( $\pm$ ) 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(<sup>3</sup>P), 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  $k/k(\text{ref})$ ) at that temperature; if it contains a temperature range, e.g. 200–500, the value in Column 4 is the Arrhenius  $A$  parameter (or  $A/A(\text{ref})$ ). Column 5 ("n") and Column 6 (" $B, B - B(\text{ref})$ "), respectively, contain, when applicable, the  $n$  and  $B$  (or  $B - B(\text{ref})$ ) parameters in the extended Arrhenius Eq.  $k = A(T/298)^n \exp(-B/T)$ .  $k(\text{ref})$ ,  $A(\text{ref})$  and  $B(\text{ref})$  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

This work was supported by the Department of Energy, Division of Basic Energy Sciences and the Office of Standard Reference Data, National Bureau of Standards. The author is grateful to Dr. John T. Herron, Director, Chemical Kinetics Data Center for his careful reading of the manuscript and frequent discussions of the subject. He is especially indebted to Mrs. Geraldine Zumwalt and Ms. Rhoda Levin for their attention to many details in the keyboarding, editing, and the preparation of the final copy of the manuscript.

### 1.8. References to the Introduction

- <sup>1</sup>R. J. Cvetanović, "Electrophilic Character of Oxygen Atoms," *Can. J. Chem.*, **38**, 1678 (1960).
- <sup>2</sup>R. J. Cvetanović, "Addition of Atoms to Olefins in the Gas Phase," *Adv. Photochem.*, **1**, 115 (1963).
- <sup>3</sup>R. J. Cvetanović, and D. L. Singleton, "Reaction of Oxygen Atoms with Olefins," *Rev. Chem. Inter.*, **5**, 183 (1984).
- <sup>4</sup>H. Yamazaki, and R. J. Cvetanović, "Collisional Deactivation of the Excited Singlet Oxygen Atoms and Their Insertion into the CH Bonds of Propane," *J. Chem. Phys.*, **41**, 3703 (1964).
- <sup>5</sup>J. Heicklen, "Gas Phase Oxidation of Perhalocarbons," *Adv. Photochem.*, **7**, 57 (1969).
- <sup>6</sup>R. E. Huie, and J. T. Herron, "Reactions of Atomic Oxygen ( $O^3P$ ) with Organic Compounds," *Prog. React. Kinet.*, **8**, 1 (1975).
- <sup>7</sup>M. C. Lin, "Dynamics of Oxygen Atom Reactions," *Adv. Chem. Phys.*, "Potential Energy Surfaces," edited by K. P. Lawley (John Wiley & Sons Ltd.) **42**, 113 (1980).
- <sup>8</sup>S.-i. Hirokami, and R. J. Cvetanović, "Reaction of Oxygen Atoms,  $O(^3P)$ , with Olefins in Liquid Nitrogen Solution at 77°K," *J. Am. Chem. Soc.*, **96**, 3738 (1974).
- <sup>9</sup>G. Boocock, and R. J. Cvetanović, "Reaction of Oxygen Atoms with Benzene," *Can. J. Chem.*, **39**, 2436 (1961).
- <sup>10</sup>G. R. H. Jones, and R. J. Cvetanović, "Reaction of Oxygen Atoms with Toluene," *Can. J. Chem.*, **39**, 2444 (1961).
- <sup>11</sup>R. J. Cvetanović, D. L. Singleton, and G. Paraskevopoulos, "Evaluations of the Mean Values and Standard Errors of Rate Constants and Their Temperature Coefficients," *J. Phys. Chem.*, **83**, 50 (1979).
- <sup>12</sup>J. T. Herron, and R. E. Huie, "Rate Constants for the Reactions of Atomic Oxygen ( $O^3P$ ) with Organic Compounds in the Gas Phase," *J. Phys. Chem. Ref. Data*, **2**, 467 (1973).

<sup>13</sup>J. Warnatz, "Rate Coefficients in the C/H/O System," in 'Combustion Chemistry', Ed. W.C. Gardiner, Jr., Springer-Verlag, 1984, p. 197.

## 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  $1.2 \times 10^{11}$ )

Temperature ( $T$ ): in kelvins (K).

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

Unit Codes for  $k$ ,  $k/k(\text{ref})$ ,  $A$ ,  $A/A(\text{ref})$ :

1 ( $s^{-1}$ ),  
 2 ( $\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$ ),  
 3 ( $\text{cm}^6\text{mol}^{-2}\text{s}^{-1}$ ),  
 1/1, 2/2, etc. (dimensionless),  
 2/1 ( $\text{cm}^3\text{mol}^{-1}$ ), etc.

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

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

$k(\text{ref})$ ,  $A(\text{ref})$  and  $B(\text{ref})$  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.

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

265

## 3. Index of Reactions and Summary of Recommended Rate Parameters

Reaction	T/K	k, A cm <sup>3</sup> mol <sup>-1</sup> s <sup>-1</sup>	n	B	k err. factor	Page
<b>O + ALKENE REACTIONS:</b>						
O + CH <sub>2</sub> =CH <sub>2</sub> → products	298	(4.40±0.56)(11)			1.2	271
O + Ethene	200-500	6.4(12)	*)	800±200	1.5	
O + CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>3</sub> + ·CHO					274	
O + Ethene						
O + CH <sub>2</sub> =CH <sub>2</sub> (EXV) → products					275	
O + Ethene(EXV)						
O + CD <sub>2</sub> =CD <sub>2</sub> → products	298	4.4(11)			1.2	275
O + Ethene-d <sub>4</sub>	200-500	6.4(12)	*)	800±200	1.5	
O + CH <sub>2</sub> =C=CH <sub>2</sub> → products	298	7.4(11)			1.2	276
O + 1,2-Propadiene	290-500	1.7(13)	*)	930±100	1.5	
O + CH <sub>2</sub> =C=CH <sub>2</sub> → H + [C <sub>3</sub> H <sub>3</sub> O]					276	
O + 1,2-Propadiene						
O + CH <sub>3</sub> CH=CH <sub>2</sub> → products	298	(2.4±0.3)(12)			1.2	276
O + 1-Propene	290-450	6.1(12)	*)	280±100	1.5	
O + CD <sub>3</sub> CD=CD <sub>2</sub> → products	298	2.4(12)			1.2	278
O + 1-Propene-d <sub>6</sub>						
O + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → 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 <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → 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 <sub>3</sub> CH=CHCH <sub>3</sub> → 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 <sub>3</sub> CH=CHCH <sub>3</sub> → 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 <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → 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 <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → 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 <sup>3</sup> mol <sup>-1</sup> s <sup>-1</sup>	n	B	k err. factor	Page
O + cis-CH <sub>3</sub> CH=CHCH <sub>2</sub> CH <sub>3</sub> → products	298	1.0(13)			1.3	285
O + cis-2-Pentene						
O + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>2</sub> → products	298	2.5(12)			1.2	285
O + 1-Butene, 3-methyl-	290-500	6.0(12)	*)	266	1.5	
O + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → products	298	3.4(13)			1.2	286
O + 2-Butene, 2-methyl-	290-400	1.7(13)		-200±200	1.5	
O + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → products	298	2.8(12)			1.3	286
O + 1-Hexene						
O + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → 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 <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> → products	298	1.27(13)			1.2	288
O + Cyclopentene	290-450	1.43(13)		40±100	1.5	
O + cy-CH=CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> → products	298	1.2(13)			1.2	288
O + Cyclohexene	290-500	1.3(13)		30±200	1.5	
O + cy-CH=C(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> → products	298	5.4(13)			1.2	289
O + Cyclohexene, 1-methyl-	290-450	1.4(13)		-400±200	1.5	
O + cy-CH=CHCH=CHCH <sub>2</sub> CH <sub>2</sub> → products	298	5.5(13)			1.2	290
O + 1,3-Cyclohexadiene	290-450	1.4(13)		-400±200	1.5	
O + C <sub>10</sub> H <sub>16</sub> → products	298	7.1(13)			1.2	290
O + d-Limonene	290-450	2.7(14)		400±200	1.5	
O + C <sub>10</sub> H <sub>16</sub> → products	298	1.7(13)			1.2	291
O + 2-Pinene	290-450	1.9(14)		710±200	1.5	
O + C <sub>10</sub> H <sub>16</sub> → products	298	1.6(13)			1.2	291
O + Nopinene	290-450	1.5(14)		660±200	1.5	
<b>O + HALOALKENE and O + KETENE REACTIONS</b>						
O + CH <sub>2</sub> =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.

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

267

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

Reaction	T/K	k, A cm <sup>3</sup> mol <sup>-1</sup> s <sup>-1</sup>	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 <sub>2</sub> -CF <sub>2</sub> → 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 <sub>2</sub> → products	298	(3.45±1.20)(11)			1.2	295
O + Ethene, trifluoro-	290-450	6.1(12)		950±150	1.5	
O + CF <sub>2</sub> =CF <sub>2</sub> → products	298	(5.88±1.35)(11)			1.2	296
O + Ethene, tetrafluoro-	290-400	1.6(12)		310±100	1.5	
O + CH <sub>2</sub> =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 <sub>2</sub> =CCl <sub>2</sub> → products	298	5.9(11)			1.2	298
O + Ethene, 1,1-dichloro-						
O + CF <sub>2</sub> =CFC1 → products	298	3.0(11)			1.2	299
O + Ethene,-	290-450	2.3(13)		1300±200	1.5	
1-chloro-1,2,2-trifluoro-						
O + CF <sub>2</sub> =CCl <sub>2</sub> → products	298	3.9(11)			1.2	299
O + Ethene,	290-450	3.5(12)		660±100	1.5	
1,1-dichloro-2,2-difluoro-						
O + CBC1=CCl <sub>2</sub> → products	298	5.9(10)			1.2	300
O + Ethene, trichloro-						
O + CH <sub>2</sub> =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 <sub>3</sub> CF=CH <sub>2</sub> → products	298	1.2(12)			1.2	300
O + 1-Propene, 2-fluoro-						
O + CH <sub>2</sub> FCH=CH <sub>2</sub> → products	298	5.0(11)			1.2	301
O + 1-Propene, 3-fluoro-						
O + CH <sub>3</sub> CH=CF <sub>2</sub> → 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	$k_A$ $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$	n	B	$k_{\text{err.}}$ factor	Page
O + $\text{CF}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$	298	2.5(10)			1.2	301
O + 1-Propene, 3,3,3-trifluoro-						
O + $\text{CF}_3\text{CF}=\text{CF}_2 \rightarrow \text{products}$	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 + $\text{CF}_2=\text{CFCF}=\text{CF}_2 \rightarrow \text{products}$	298	2.2(11)			1.2	302
O + 1,3-Butadiene,						
1,1,2,3,4,4-hexafluoro-						
O + $\text{CH}_2=\text{CHCH}_2\text{Cl} \rightarrow \text{products}$	298	6.1(11)			1.2	303
O + 1-Propene, 3-chloro-						
O + $\text{CH}_3\text{C}(\text{CF}_3)=\text{CH}_2 \rightarrow \text{products}$	298	(2.26±0.29)(11)			1.2	303
O + 1-Propene, 2-trifluoromethyl-	200-450	5.8(12)		942±200	1.5	
O + $\text{CH}_2\text{FCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$	298	1.4(12)			1.2	304
O + 1-Butene, 4-fluoro-						
O + $\text{CH}_3\text{CH}_2\text{CF}=\text{CF}_2 \rightarrow \text{products}$	298	(2.45±0.05)(12)			1.2	304
O + 1-Butene, 1,1,2-trifluoro-						
O + $\text{CH}_2=\text{CO} \rightarrow \text{adduct(EXV)}$	298	(2.37±0.79)(11)			1.2	304
O + Ethenone (Ketene)	230-449	1.8(12)		680±200	1.5	
O + $\text{CH}_3\text{CH}=\text{CO} \rightarrow \text{adduct(EXV)}$	298	(6.8±0.2)(12)			1.2	305
O + 1-Propen-1-one	230-449	2.9(12)		-250±100	1.5	
O + $\text{CH}_3\text{CH}_2\text{CH}=\text{CO} \rightarrow \text{adduct(EXV)}$	298	(7.34±0.84)(12)			1.2	305
O + 1-Buten-1-one	230-449	3.2(12)		-220±100	1.5	
O + $(\text{CH}_3)_2\text{C}=\text{CO} \rightarrow \text{adduct(EXV)}$	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	
<b>O + ALKYNE REACTIONS</b>						
O + $\text{CH}=\text{CH} \rightarrow \text{products}$	298	9.0(10)			1.2	307
O + Ethyne	250-1300	1.6(13)		1550±100	1.5	
O + $\text{CH}=\text{CH} \rightarrow \text{CO} + \text{CH}_2$	300-2500	2.1(12)	1.5	850	2	309
O + Ethyne						
O + $\text{CH}=\text{CH} \rightarrow \text{H} + \text{CH}=\text{C=O}$	300-600	9.0(12)		2300±300	1.5	309
O + Ethyne	1000-2500	4.3(14)		6100	3	

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

269

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

Reaction	T/K	k, A cm <sup>3</sup> mol <sup>-1</sup> s <sup>-1</sup>	n	B	k err. factor	Page
O + CD≡CD → products	298	8.6(10)			1.2	310
O + Ethyne-d2						
O + CH <sub>3</sub> C≡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 <sub>3</sub> C≡CH → H + [C <sub>3</sub> H <sub>3</sub> O]	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 <sub>2</sub> =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 <sub>3</sub> CH <sub>2</sub> C≡CH → CO + CH <sub>3</sub> CH=CH <sub>2</sub>	298	1.2(12)			1.2	312
O + 1-Butyne	298-1300	2.0(13)		835±100	1.5	
O + CH <sub>3</sub> C≡CCH <sub>3</sub> → CO + CH <sub>3</sub> CH=CH <sub>2</sub>	298	2.9(12)			1.2	312
O + 2-Butyne	290-360	6(13)		900±300	1.5	
O + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CH → CO(EXV) + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH:	298	4.5(11)			1.5	313
O + 1-Pentyne						
O + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CH → CO(EXV) + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH:	298	3.3(11)			1.5	313
O + 1-Hexyne						
O + AROMATIC HYDROCARBON REACTIONS						
O + C <sub>6</sub> H <sub>6</sub> → products	298	(1.22±0.29)(10)			1.3	314
O + Benzene	298-600	1.52(13)		2130±200	2	
O + C <sub>6</sub> D <sub>6</sub> → products	298	*)			1.3	315
O + Benzene-d6	376-944	*)		*)	2	
*) Same as for O+C <sub>6</sub> H <sub>6</sub>						
O + C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> → products	298	5.0(10)			1.4	315
O + Benzene, methyl-	298-932	1.63(13)		1720±200	2	
O + C <sub>6</sub> H <sub>5</sub> CD <sub>3</sub> → 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 <sup>3</sup> mol <sup>-1</sup> s <sup>-1</sup>	n	B	k err. factor	Page
O + C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>3</sub> → products	298	6(10)				317
O + Benzene, ethyl-						
O + o-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> → products	298	1.2(11)			1.3	317
O + o-Xylene	298-600	(1.5±1.2)(13)		1382±300	2	
O + o-CD <sub>3</sub> C <sub>6</sub> D <sub>4</sub> CD <sub>3</sub> → products	298	1.2(11)			1.3	318
O + o-Xylene-d10	298-600	2.1(13)		1550	2	
O + m-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> → products	298	2.4(11)			1.3	318
O + m-Xylene	298-600	(1.5±1.1)(13)		1216±200	2	
O + m-CD <sub>3</sub> C <sub>6</sub> D <sub>4</sub> CD <sub>3</sub> → 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 <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> → products	298	1.2(11)			1.2	319
O + p-Xylene	298-600	(1.57±1.10)(13)		1409±185	2	
O + C <sub>6</sub> H <sub>5</sub> C(CH <sub>3</sub> ) <sub>3</sub> → products	298	4(10)			2	320
O + Benzene, t-butyl-						
O + 1,2,3-(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>3</sub> → 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 <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>3</sub> → 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 <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>3</sub> → products	298	1.6(12)			2	321
O + Benzene, 1,3,5-trimethyl-	298-600	6.0(12)		400±200	2	
O + C <sub>6</sub> H <sub>5</sub> N → products	298	4.3(10)			2	321
O + Pyridine	300-500	2.9(12)		1260±300	2	
O + C <sub>6</sub> H <sub>5</sub> Cl → products	298	3(11)			3	322
O + Benzene, chloro-						
O + C <sub>6</sub> H <sub>5</sub> F → products	298	8(9)			3	322
O + Benzene, fluoro-						
O + C <sub>6</sub> H <sub>5</sub> CF <sub>3</sub> → products	298	3.5(9)			3	322
O + Benzene, trifluoromethyl-						

## 4. Tables of Chemical Kinetic Data

Table 4.1. Data for O(<sup>3</sup>P) 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 factor
<b>O + CH<sub>2</sub>=CH<sub>2</sub> → products</b>						
Oxygen atom + Ethene						
58 KAU	EX	296	5(10)			2
Discharge flow-O+NO chemiluminescence.						
Overall k is "about" 5x10 <sup>10</sup> cc/mol.sec.						
60 CVE2	RL	298-400	1.01		1011	2/2
k/k <sub>ref</sub> 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(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>2</sub>=CH<sub>2</sub> → products -- Continued</b>							
72 ATK/CVE Phase shift-O+NO chemiluminescence. Updated in 76 SIN/CVE.	EX	298-4/4	8.1(12)		976±50	2	
71 STU/NIK Flash photolysis-NO+O chemiluminescence. *) Stated error limits: +5%, -15%.	EX	300	(3.79± *) (11)			2	
72 STU/NIK Flash photolysis-NO+O and CO+O chemiluminescence.	EX	298±2	(3.76±0.38)(11)			2	
72 DAV/HUI Discharge flow-Mass spectrometry.	EX	298	5.22(11)			2	
Flash photolysis-Kinetic absorption.	EX	298	(5.30±0.27)(11)			2	
Flash photolysis-Resonance fluorescence.	EX	298	(5.08±0.30)(11)			2	
Flash photolysis-Resonance fluorescence.	EX	232-500	(3.26±0.18)(12)	569±16		2	
73 KUR/HUI Flash photolysis-Resonance fluorescence.	EX	298	(4.79±0.48)(11)			2	
73 HER/HUI SE 298 SE 200-500	SE	298	4.9(11)	565	2	1.2	
74 PUR/ATK Phase shift-O+NO chemiluminescence. P = 30-90 torr.	EX	298	(4.32±0.45)(11)			2	
74 ATK/PIT2 Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.	EX	300	(4.00±0.40)(11)			2	
74 ATK/PIT1 Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.	EX	298-392	3.37(12)	639±100		2	
74 SLA/PRU Discharge flow-Mass spectrometry. P=0.78-2.14 torr.	EX	298	(4.64±0.22)(11)			2	
74 MCC Ref. Rn: O + Isobutene → products k/k <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O <sub>2</sub> photolysis at 184.9 nm. Current normalized value (86 CVE): k=4.28(11)	RL	298±5	0.042±0.010			2/2	
76 SIN/CVE Phase shift-O+NO chemiluminescence.	EX	298	(4.23±0.10)(11)			2	
	EX	298-486	(6.98±0.89)(12)	845±47		2	

Table 4.1. Data for O(<sup>3</sup>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 factor
<b>O + CH<sub>2</sub>=CH<sub>2</sub> → products -- Continued</b>						
76 MAN/BRA  Flash-photolysis. Resonance-fluorescence. P(tot) = 5 torr.	EX	298	(4.5±0.2)(11)			2
77 ATK/PIT1  Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.	EX	298	(4.58±0.46)(11)			2
	EX	298-439	5.56(12)	742±100		2
80 SUG/ISH  Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.	EX	296±2	(6.0±1.2)(11)			2
82 NIC/RAV  Flash-photolysis. Resonance-fluorescence. O generated by flash-photolysis of O <sub>2</sub> . [O] ~ (2-4)(10) molec.cm <sup>-3</sup> . P(Ar)=100 torr. [CH <sub>2</sub> =CH <sub>2</sub> ] = (0.01-2.0)(15) molec.cm <sup>-3</sup> .	EX	298	(4.32±0.44)(11)			2
	EX	298-500	(7.35±3.73)(12)	870±190		2
82 NIC/RAV  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  Discharge flow-mass spectrometry with molecular beam sampling. Large excess of O.	EX	298-736	*)			2
*) Effect of pressure (0.5-5 torr He) on k: Values of k×10 <sup>-11</sup> 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  Selected as the mean of a chosen set of data.	SE	298	(4.58±0.16)(11)			2
84 PER1  O atoms from F <sub>2</sub> excimer laser photolysis (157 nm) of O <sub>2</sub> & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=4.59(11) (calcd. from Arrhs. Eq.)	EX	294	(4.55±0.46)(11)			2
	EX	294-820	4.63(12)	0.63 689		2

Table 4.1. Data for O(<sup>3</sup>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 factor
<b>O + CH<sub>2</sub>=CH<sub>2</sub> → products -- Continued</b>						
84 PER2 O atoms from F <sub>2</sub> excimer laser photolysis (157 nm) of O <sub>2</sub> & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=4.96(11) (calcd. from Arrhs. Eq.)	EX	260-860	2.87(12)	1.0	523	2
84 BRO/STU O atoms from H <sub>2</sub> laser photolysis of NO, monitored by O+NO chemiluminescence.	EX	298	(3.98±0.24)(11)			2
	EX	197-372	(5.06±1.63)(12)		757±120	2
86 CVE Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).	RN	298	(4.32±0.25)(11)			2
	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 *) 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).	RE	200-500	6.4(12)	*)	800±200	2 1.5
82 TEM/WAG Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products	RL	298	0.35-0.60			2/2
Reaction of O with CH <sub>2</sub> =CH <sub>2</sub> 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 <sub>ref</sub> ) is in the range 0.35-0.60.						

Table 4.1. Data for O(<sup>3</sup>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 factor
<b>O + CH<sub>2</sub>=CH<sub>2</sub>(EXV) → products</b>						
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 calcu- lated for thermal heating by the laser alone.						
<b>O + CD<sub>2</sub>=CD<sub>2</sub> → products</b>						
Oxygen atom + Ethene-d <sub>4</sub>						
72 STU/NIK	EX	298±2	(3.37±0.34)(11)			2
Flash photolysis-NO+O & CO+O chemilumi- nescence.						
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
Flash-photolysis. Resonance-fluorescence. O generated by flash-photolysis of O <sub>2</sub> . [O] ~ (2-4)(10) molec.cm <sup>-3</sup> . P(Ar)=100 torr [CD <sub>2</sub> =CD <sub>2</sub> ] = (0.01-2.0)(15) molec.cm <sup>-3</sup> .						
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); 585K: (1.6±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(<sup>3</sup>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 corr. factor
<b>O + CH<sub>2</sub>=C=CH<sub>2</sub> → products</b>							
Oxygen atom + 1,2-Propadiene (Allene)							
77 ATK/PITZ	EX	297	(6.94±0.66)(11)			2	
	EX	297-439	1.23(13)		883±100	2	
Flash-photolysis. NO <sub>2</sub> 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 <sub>2</sub> O 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.							
<b>O + CH<sub>2</sub>=C=CH<sub>2</sub> → H + [C<sub>3</sub>H<sub>5</sub>O]<sup>·</sup></b>							
A path in the rxn. O + CH <sub>2</sub> =C=CH <sub>2</sub> → products							
80 ALE/ARU	EX	295-860	6.6(12)		1535±150	2	
Resonance-fluorescence.							
k(298K)=3.8(10) (calcd. from Arrhs. Eq.)							
<b>O + CH<sub>3</sub>CH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene							
58 CVE	RL	298	0.23			2/2	
k/k <sub>ref</sub> from products in competing expts.							
Ref. Rxn: 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(<sup>3</sup>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
<b>O + CH<sub>3</sub>CH=CH<sub>2</sub> → products -- Continued</b>							
73 HER/HUI	SE	298	2.2(12)			2	1.2
	SE	200-500	2.5(12)	38		2	1.2
74 FUR/ATK Phase shift-O+NO chemiluminescence.	EX	298	(2.02±0.17)(12)			2	
74 ATK/PIT2 Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.	EX	300	(2.01±0.22)(12)			2	
74 ATK/PIT1 Phase shift-O+NO chemiluminescence. Error shown is estimated "overall" error.	EX	208-302	2.08(12)	0±150		2	
74 MCC Ref. Rn: O + Isobutene → products k/k <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O <sub>2</sub> photolysis at 184.9 nm. Current normalized value (86 CVE): k=2.04(12)	RL	298±5	0.20±0.05			2/2	
75 GAF/ATK1 Product yields in competing expts. Ref. Rn: O + Cyclopentene → products Normd. k=2.10(12); update (86 CVE) 2.30(12).	RL	296±2	0.181±0.010			2/2	
76 SIN/CVE Phase shift-O+NO chemiluminescence.	EX	298	(2.28±0.08)(12)			2	
	EX	298-483	(7.58±0.42)(12)	363±20		2	
77 ATK/PIT1 Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.	EX	298	(2.69±0.27)(12)			2	
	EX	298-439	6.32(12)	259±100		2	
77 MIC/LEE Discharge flow-Resonance fluorescence. P = 0.76-2.5 torr.	EX	298	(2.38±0.25)(12)			2	
78 KOH O atoms from H <sub>2</sub> laser photolysis of NO, monitored by O+NO chemiluminescence.	EX	298	(2.03±0.11)(12)			2	
	EX	200-353	(3.61±0.42)(12)	168±36		2	
80 SUG/ISH Pulse-radicalysis. Resonance-absorption P = 50-950 torr.	EX	296±2	(2.83±0.18)(12)			2	
82 BIE/HAR Discharge-flow system. Photoionization mass-spec. P(Tot) ~ 2 torr.	EX	298	(2.65±0.36)(12)			2	
84 CVE/SIN Selected as the mean of a chosen set of data.	SE	298	(2.44±0.12)(12)			2	

Table 4.1. Data for O(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>3</sub>CH=CH<sub>2</sub> → products -- Continued</b>							
84 PER1	EX	293	(2.69±0.27)(12)			2	
	EX	258-861	4.42(11)	2.56	-569	2	
O atoms from F <sub>2</sub> excimer laser photolysis (at 157 nm) of O <sub>2</sub> 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 <sub>2</sub> 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).							
<b>O + CD<sub>3</sub>CD=CD<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene-d <sub>6</sub>							
84 PER1	EX	285	(2.77±0.28)(12)			2	
	EX	285-817	3.73(11)	2.53	-609	2	
O atoms from F <sub>2</sub> excimer laser photolysis (at 157 nm) of O <sub>2</sub> 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

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

279

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 factor
<b>O + <math>CH_2=CHCH=CH_2 \rightarrow</math> products</b>						
Oxygen atom + 1,3-Butadiene						
60 CVE/DOY	RL	299-400	1.14	103		2/2
k/k <sub>ref</sub> 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 <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins.						
O from O <sub>2</sub> 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 <sub>2</sub> chemiluminescence. Error in B is "estimated overall" error.						
79 NIP/SIN	EX	299	(1.31±0.04)(13)		2	
Modulated Hg-sensitized N <sub>2</sub> O 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						
Recommended values of Arrhenius A and B	RE	298	(1.10±0.10)(13)		2	1.2
	RE	290-500	1.4(13)	40±150	2	1.5

Table 4.1. Data for O(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Butene							
60 CVE2	RL	299-399	0.74			404	2/2
k/k <sub>ref</sub> 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 k×10 <sup>-12</sup> increase from 1.95(190K) to 3.57(491K).							
Authors assume two simultaneous processes: O-addition (A=(2.2±1.1)(12); B=25±106) 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(-980/T) (The 1st term is assumed to be addition and the 2nd H-abstraction by O atoms. For con- trary 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 <sub>ref</sub> obtained from ratios of NO+O chemi- luminescence signals with different olefins.							
O from O <sub>2</sub> 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	298-424	(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(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → products -- Continued</b>							
80 SUG/ISH Pulse-radiolysis. Resonance-absorption P = 50-950 torr.	EX	296±2	(2.8±0.3)(12)			2	
84 CVE/SIN Selected as the mean of a chosen data set.	SE	298	(2.55±0.07)(12)			2	
84 PER2 O atoms from F <sub>2</sub> excimer laser photolysis (197 nm) of O <sub>2</sub> & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=2.62(12) (calcd. from Arrhs. Eq.)	EX	260-860	4.45(11)	2.34	-528	2	
84 BRO/STU O atoms from H <sub>2</sub> laser photolysis of NO, monitored by OH+NO chemiluminescence. Curved Arrhenius plot. For T<273K B=186. For T>273K B=403.	EX	298	(2.43±0.07)(12)			2	
	EX	197-372	(5.54±1.81)(12)		241±60	2	
86 CVE Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).	RN	298	(2.43±0.08)(12)			2	
	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 *) 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)	RE	290-450	8.1(12)	*)	350±100	2	1.5
<b>O + cis-CH<sub>3</sub>CH=CHCH<sub>3</sub> → products</b>							
Oxygen atom + cis-2-Butene	RL	300	0.001±0.014			2/2	
60 CVE1 k/k <sub>ref</sub> from products in competing expts. Ref. Rn: O + Cyclopentene → products Current normalized value (86 CVE): k=1.02(13)	EX	298	(1.03±0.04)(13)			2	
	EX	268-443	(5.84±0.58)(12)		-161±32	2	
73 DAV/HUI Flash photolysis-Resonance fluorescence.	SE	298	1.0(13)			2	
73 HER/HUI	SE	200-500	5.9(12)		-165	2	1.2

Table 4.1. Data for O(<sup>3</sup>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
<b>O + cis-CH<sub>3</sub>CH=CHCH<sub>3</sub> → products -- Continued</b>							
74 FUR/ATK Phase shift-O+NO chemiluminescence. P = 30-50 torr.	EX	298	(9.00±1.76)(12)			2	
74 MCC Ref. Rn: O + Isobutene → products k/k <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O <sub>2</sub> photolysis at 184.9 nm. Current normalized value (86 CVE): k=8.06(12)	RL	298±5	0.79±0.25			2/2	
76 SIN/CVE Phase shift-O+NO chemiluminescence.	EX	298	(1.06±0.04)(13)			2	
	EX	298-484	(6.68±0.23)(12)		-135±13	2	
77 ATK/PIT1 Flash photolysis-Chemiluminescence. Error in B is "estimated overall" error.	EX	298	(1.09±0.11)(13)			2	
	EX	298-439	7.29(12)		-118±100	2	
80 SUG/ISH Pulse-radiolysis. Resonance-absorption. P = 50-950 torr.	EX	296±2	(1.2±0.2)(13)			2	
84 CVE/SIN Selected as the mean of a chosen set of data.	SE	298	(1.06±0.02)(13)			2	
84 PER2 O atoms from F <sub>2</sub> excimer laser photolysis (157 nm) of O <sub>2</sub> & NO; monitored by NO+O chemiluminescence. Curved Arrhenius plot. k(298K)=1.09(13) (calcd. from Arrhs. Eq.)	EX	260-860	5.66(11)	2.07 -881		2	
86 CVE Derived from relative k data (60 CVE1) using for Cyclopentene k=1.27(13).	RN	300	(1.02±0.02)(13)			2	
	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(<sup>3</sup>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 k err. units factor
<b>O + trans-CH<sub>3</sub>CH=CHCH<sub>3</sub> → products</b>						
Oxygen atom + trans-2-Butene						
60 CVE1	RL	300	0.951±0.042			2/2
k/k <sub>ref</sub> 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 <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins.						
O from O <sub>2</sub> 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.						
0 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 <sub>2</sub> excimer laser photolysis (157 nm) of O <sub>2</sub> & 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(<sup>3</sup>P) Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/ref, A, A/A(ref)	n	B, B-B(ref)	k, A units factor
<b>O + (CH<sub>3</sub>)<sub>2</sub>C=CH<sub>2</sub> → products</b>						
Oxygen atom + 1-Propene, 2-methyl- (Isobutene)						
60 CVE2	RL	299-403	0.67	-65	2/2	
k/k <sub>ref</sub> 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/PITI	EX	298	(9.22±0.90)(12)	2		
EX 298-439 1.05(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 <sub>2</sub> excimer laser photolysis (157 nm) of O <sub>2</sub> & 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(<sup>3</sup>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 factor
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → products</b>						
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 <sub>2</sub> +M) of 55 BEN/AXW. O-atoms from NO <sub>2</sub> 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
<b>O + cis-CH<sub>3</sub>CH=CHCH<sub>2</sub>CH<sub>3</sub> → products</b>						
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 <sub>2</sub> +M) of 55 BEN/AXW. O-atoms from NO <sub>2</sub> photolysis at 366 nm.						
59 CVE	RL	298	0.75			2/2
k/k <sub>ref</sub> : 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
<b>O + (CH<sub>3</sub>)<sub>2</sub>CHCH=CH<sub>2</sub> → products</b>						
Oxygen atom + 1-Butene, 3-methyl-						
74 MCC	RL	298±5	0.22±0.05			2/2
Ref. Rn: O + Isobutene → products k/k <sub>ref</sub> obtained from ratios of NO+O chemiluminescence signals with different olefins. O from O <sub>2</sub> 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
Phase shift-O+NO chemiluminescence.	EX	298-484	(6.02±0.44)(12)	266±26		2
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(<sup>3</sup>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
<b>O + (CH<sub>3</sub>)<sub>2</sub>CHCH=CH<sub>2</sub> → products -- Continued</b>							
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)							
<b>O + (CH<sub>3</sub>)<sub>2</sub>C=CHCH<sub>3</sub> → products</b>							
Oxygen atom + 2-Butene, 2-methyl-							
60 CVE2	RL	298-400	1.18		-240	2/2	
k/k <sub>ref</sub> 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
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Hexene							
60 CVE1	RL	299	0.218±0.004			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + Cyclopentene → products							
Current normalized value (86 CVE): k=2.77(12)							

**CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS**

287

Table 4.1. Data for O(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → products -- Continued</b>							
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
<b>O + (CH<sub>3</sub>)<sub>2</sub>C=C(CH<sub>3</sub>)<sub>2</sub> → products</b>							
Oxygen atom + 2-Butene, 1,2-Dimethyl-(Tetramethylethylene)							
60 CVE2	RL	300-393	1.25		-300	2/2	
k/k <sub>ref</sub> 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(<sup>3</sup>P) Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/ref, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
<b>O + cy-CH=CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub> → products</b>							
Oxygen atom + Cyclopentene							
60 CVE2	RL	299-403	1.49	65		2/2	
k/k <sub>ref</sub> 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 <sub>ref</sub> 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=5.5(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 <sub>iso-Butene</sub> = 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 <sub>Propene</sub> = 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							
Recommended values of Arrhenius A and B assuming linear Arrhenius plot for 290-450K.							
0 + cy-CH=CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> → products	RE	298	1.27(13)		2	1.2	
Oxygen atom + Cyclohexene							
60 CVE2	RL	298-400	0.89	-7	2/2		
k/k <sub>ref</sub> 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(<sup>3</sup>P) Reactions with Alkenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<b>O + cy-CH=CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub> → products -- Continued</b>							
82 WAS/TAK	EX	298	(1.20±0.03)(13)			2	
Reaction of Cyclohexene with O atoms in a fast-flow reactor. O atoms generated by a microwave-discharge in a He-O <sub>2</sub> mixture. Mass-spectrometry. P(Tot) = 3.7 torr. P(Cyclohexene) = 0.004-0.012 mtorr. P(O <sub>2</sub> ) <sub>0</sub> = 0.266-0.560 mtorr,							
86 CVE	RN	298	(1.15±0.06)(13)			2	
Derived from relative k data (60 CVE2) using for Cyclopentene k=1.27(13).							
	RN	298-400	1.27(13)		33	2	
Derived from relative k data (60 CVE2) using for Cyclopentene A=1.43(13), B=40.							
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	
<b>O + cy-CH=C(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub> → products</b>							
Oxygen atom + Cyclohexene, 1-methyl-							
75 GAF/ATK2	RL	296-423	0.95	-453±70	2/2		
k/k <sub>ref</sub> 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)							
86 CVE	RN	296	(5.35±0.22)(13)		2		
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene k=1.27(13).							
	RN	296-423	1.36(13)	-413	2		
Derived from relative k data (75 GAF/ATK2) using for Cyclopentene A=1.43(13), B=40.							
Recommended value of k	RE	296	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(<sup>3</sup>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	k err. units factor
<b>O + cy-CH=CHCH=CHCH<sub>2</sub>CH<sub>2</sub> → products</b>							
Oxygen atom + 1,3-Cyclohexadiene							
75 GAF/ATK2	RL	296-423	0.92		-448±55	2/2	
k/k <sub>ref</sub> 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	RE	290-450	1.4(13)		-400±200	2	1.5
assuming linear Arrhenius plot for 290-450K.							
<b>O + C<sub>10</sub>H<sub>16</sub> → products</b>							
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 <sub>ref</sub> 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	RE	290-450	2.7(14)		400±200	2	1.5
assuming linear Arrhenius plot for 290-450K.							

Table 4.1. Data for O(<sup>3</sup>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
<b>O + C<sub>10</sub>H<sub>16</sub> → products</b>							
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 <sub>ref</sub> 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=1.02(14), B=714, k(208)=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
 <b>O + C<sub>10</sub>H<sub>16</sub> → products</b>							
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 <sub>ref</sub> 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(<sup>3</sup>P) 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 factor	err.
<b>O + CH<sub>2</sub>=CHF → products</b>							
Oxygen atom + Ethene, fluoro- (Fluoroethylene)							
71 MOS	RL	296	0.38				2/2
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
O from Hg-photosensitized decomprn. of N <sub>2</sub> O. 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 <sub>ref</sub> from products in competing expts.: 298K: 0.409; 420K: 0.516. Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decomprn. of N <sub>2</sub> O. 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 decomprn. of N <sub>2</sub> O.							
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 <sub>2</sub> =CH <sub>2</sub> k=4.40(11).							
	RN	298	1.80(11)				2
Derived from relative k (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).							
	RN	298-420	6.02(12)		1043		2
Derived from relative k's (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> A=6.40(12), B=800.							

Table 4.2. Data for O(<sup>3</sup>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
<b>O + CH<sub>2</sub>=CHF → products -- Continued</b>							
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
<b>O + CHF=CHF → products</b>							
Oxygen atom + Ethene, 1,2-difluoro-							
72 HUI/HER2 Discharge flow-Mass spectrometry.	EX	307	(2.70±0.34)(11)			2	
73 HER/HUI	SE	307	2.7(11)			2	1.3
Recommended value of k	RE	298	2.7(11)			2	1.3
<b>O + cis-CHF=CHF → products</b>							
Oxygen atom + Ethene, 1,2-difluoro-, (Z)-							
71 MOS k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. Normalized absolute k=1.5(11) (73 HER/HUI). Current update (86 CVE) k=1.41(11)	RL	296	0.32			2/2	
74 JON/MOS k/k <sub>ref</sub> from products in competing expts.: 298K: 0.309; 420K: 0.452. Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decompr. of N <sub>2</sub> O. Current normalized values (86 CVE): k(298)=1.36(11), A=7.17(12), B=1173	RL	298-420	1.12		373		2/2
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	2.22(11)			2	
86 CVE Derived from relative k (71 MOS) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	296	1.41(11)			2	
	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 <sub>2</sub> =CH <sub>2</sub> 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(<sup>3</sup>P) Reactions with Halopalkenes 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 factor	k err.
<b>O + trans-CHF=CHF → products</b>							
Oxygen atom + Ethene, 1,2-difluoro-, (E)-							
71 MOS	RL	296	0.54				2/2
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decomn. of N <sub>2</sub> O. 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				2/2
k/k <sub>ref</sub> from products in competing expts.: 298K: 0.564; 420K: 0.713. Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products Measured: epoxide & aldehyde from Ref. Rn. O from Hg-photosensitized decomn. of N <sub>2</sub> O. 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 <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	298	2.48(11)				2
Derived from relative k (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	298-420	8.1(12)				1037
Derived from relative k's (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> 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
<b>O + CH<sub>2</sub>=CF<sub>2</sub> → products</b>							
Oxygen atom + Ethene, 1,1-difluoro-							
71 MOS	RL	296	0.22				2/2
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decomn. of N <sub>2</sub> O. Normalized absolute k=1.1(11) (73 HER/HUI). Current update (86 CVE) k=9.68(10)							
72 HUI/HER2	EX	307	(2.18±0.18)(11)				2
Discharge flow-Mass spectrometry.							
73 HER/HUI	SE	307	2.2(11)				2 1.3

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

295

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 factor
<b><math>O + CH_2=CF_2 \rightarrow</math> products -- Continued</b>						
74 JON/MOS	RL	298-420	0.65	321		2/2
k/k <sub>ref</sub> from products in competing expts.: 298K: 0.215; 420K: 0.299.						
Ref. Rn: $O + CH_2=CH_2 \rightarrow$ products						
Measured: epoxide & aldehyde from Ref. Rn.						
$O$ from Hg-photosensitized decompr. of $N_2O$ .						
Current normalized values (86 CVE):						
k(298)=0.46(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
<b><math>O + CHF=CF_2 \rightarrow</math> products</b>						
Oxygen atom + Ethene, trifluoro-						
71 MOS	RL	296	0.57			2/2
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: $O + CH_2=CH_2 \rightarrow$ products						
$O$ from Hg-photosensitized decompr. 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	0.06	147		2/2
k/k <sub>ref</sub> from products in competing expts.: 298K: 0.569; 420K: 0.569.						
Ref. Rn: $O + CH_2=CH_2 \rightarrow$ products						
Measured: epoxide & aldehyde from Ref. Rn.						
$O$ from Hg-photosensitized decompr. 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(<sup>3</sup>P) Reactions with Halopalkenes 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 factor	k err.
<b>O + CHF=CF<sub>2</sub> → products -- Continued</b>							
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 <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	296	2.51(11)				2
	RN	296	2.50(11)				2
Derived from relative k (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	298-420	6.14(12)	947			2
Derived from relative k's (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> A=6.40(12), B=800.							
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
<b>O + CF<sub>2</sub>=CF<sub>2</sub> → products</b>							
Oxygen atom + Ethene, tetrafluoro-							
65 SAU/HEI k/k <sub>ref</sub> from products in competing expts. Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. 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 <sub>ref</sub> from products in competing expts: 1.10(297K), 0.856(343K), 0.735(398K) Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. 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 <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from flash photolysis of NO <sub>2</sub> . CF <sub>2</sub> 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(<sup>3</sup>P) Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
<b>O + CF<sub>2</sub>=CF<sub>2</sub> → products -- Continued</b>						
71 MOS	RL	296	1.60			2/2
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products						
O from Hg-photosensitized decomn. of N <sub>2</sub> O.						
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 <sub>ref</sub> from products in competing expts. 298K: 1.707; 420K: 1.338.						
Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products						
Measured: epoxide & aldehyde from Ref. Rn.						
O from Hg-photosensitized decomn. of N <sub>2</sub> O.						
Current normalized values (86 CVE):						
k(298)=7.51(11), A=4.99(12), B=555						
75 GER/MOI	RL	300-406	0.11±0.06	-1258±20		2/2
k/k <sub>ref</sub> from products in competing expts. using a modified "diffusion flame" method: Ref. Rn: O + CH≡CH → products						
Taken k <sub>ref</sub> =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 <sub>2</sub> ( <sup>3</sup> B <sub>1</sub> ) emission.						
O from Hg-photosensitized decomn. of N <sub>2</sub> O.						
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/HEI) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	297	4.84(11)			2
Derived from relative k (66 SAU/HEI) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	297-398	1.43(12)	322±100		2
Derived from relative k's (66 SAU/HEI) using for CH <sub>2</sub> =CH <sub>2</sub> A=6.40(12), B=800.	RN	296	4.62(11)			2
Derived from relative k (69 TYE) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).	RN	296	7.04(11)			2
Derived from relative k (71 MOS) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).						

Table 4.2. Data for O(<sup>3</sup>P) Reactions with Halocalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<b>O + CF<sub>2</sub>=CF<sub>2</sub> → products -- Continued</b>							
86 CVE	RN	298	7.51(11)			2	
		298-420	4.99(11)	555		2	
Derived from relative k's (74 JON/MOS) using for CH <sub>2</sub> =CH <sub>2</sub> 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
<b>O + CH<sub>2</sub>=CHCl → products</b>							
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 decompr. of N <sub>2</sub> O.							
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
<b>O + CH<sub>2</sub>=CCl<sub>2</sub> → products</b>							
Oxygen atom + Ethene, 1,1-dichloro-							
75 SAN/HEI	RL	298	1.0			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CF <sub>2</sub> =CF <sub>2</sub> → products Measured: CO and CF <sub>2</sub> O from Ref. Rn. O from Hg-photosensitized decompr. of N <sub>2</sub> O. Current normalized k=5.88(11) (86 CVE).							

## CHEMICAL KINETIC DATA FOR REACTIONS OF OXYGEN WITH HYDROCARBONS

299

Table 4.2. Data for O(<sup>3</sup>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
<b>O + CH<sub>2</sub>=CCl<sub>2</sub> → products -- Continued</b>							
86 CVE	RN	298	5.88(11)			2	
Derived from relative k (75 SAN/HEI) using for CF <sub>2</sub> =CF <sub>2</sub> k=5.88(11).							
Recommended value of k	RE	298	5.9(11)			2	1.2
<b>O + CF<sub>2</sub>=CFCl → products</b>							
Oxygen atom + Ethene, 1-chloro-1,2,2-trifluoro-							
69 TYE	RL	296-419	14.4		989	2/2	
k/k <sub>ref</sub> from products in competing expts.: 0.51(296K), 1.36(419K)							
Ref. Rn: O + CF <sub>2</sub> =CF <sub>2</sub> → products							
O from flash photolysis of NO <sub>2</sub> . CF <sub>2</sub> 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 <sub>2</sub> =CF <sub>2</sub> 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	
<b>O + CF<sub>2</sub>=CCl<sub>2</sub> → products</b>							
Oxygen atom + Ethene, 1,1-dichloro-2,2-difluoro-							
69 TYE	RL	296-419	2.20		352	2/2	
k/k <sub>ref</sub> from products in competing expts.: 0.67(296K), 0.95(419K)							
Ref. Rn: O + CF <sub>2</sub> =CF <sub>2</sub> → products							
O from flash photolysis of NO <sub>2</sub> . CF <sub>2</sub> 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 <sub>2</sub> =CF <sub>2</sub> 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(<sup>3</sup>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	k err. units factor
<b>O + CCl=CCL<sub>2</sub> → products</b>							
Oxygen atom + Ethene, trichloro-							
74 SAN/HEI	RL	298	0.10			2/2	
k/k <sub>ref</sub> from CO yields in competing expts., O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
Ref. Rn: O + CF <sub>2</sub> =CF <sub>2</sub> → 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 <sub>2</sub> =CF <sub>2</sub> k=5.88(10).							
Recommended value of k	RE	298	5.9(10)			2	1.2
<b>O + CH<sub>2</sub>=CHBr → products</b>							
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 <sub>2</sub> O.							
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
<b>O + CH<sub>3</sub>CF=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene, 2-fluoro-							
69 MOS/JEN	RL	296	0.46			2/2	
k/k <sub>ref</sub> from products in competing expts.:							
Ref. Rn: O + 1-Butene → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>2</sub>FCH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene, 3-fluoro-							
69 MOS/JEN	RL	296	0.21			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + 1-Propene → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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
<b>O + CH<sub>3</sub>CH=CF<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene, 1,1-difluoro-							
69 MOS/JEN	RL	296	0.45			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + 1-Propene → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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
<b>O + CF<sub>3</sub>CH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene, 3,3,3-trifluoro-							
69 MOS/JEN	RL	296	0.057			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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 <sub>2</sub> =CH <sub>2</sub> k=4.40(11).							
Recommended value of k	RE	298	2.5(10)			2	1.2

Table 4.2. Data for O(<sup>3</sup>P) Reactions with Halopkenes 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	k err. units factor
<b>O + CF<sub>3</sub>CF=CF<sub>2</sub> → products</b>							
Oxygen atom + 1-Propene, 1,1,2,3,3,3-hexafluoro-(perfluoropropylene)							
66 SAU/HEI2	RL 207		0.034			2/2	
k/k <sub>ref</sub> from products in competing expts.							
Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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 <sub>ref</sub> from products in competing expts.: 0.0357(297K), 0.0385(343K), 0.0488(398K)							
Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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 (66 SAU/HEI2) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).							
RN 298			1.57(10)			2	
Derived from relative k (66 SAU/HEI) using for CH <sub>2</sub> =CH <sub>2</sub> k=4.40(11).							
RN 297-398			7.81(11)		1166	2	
Derived from relative k's (66 SAU/HEI) using for CH <sub>2</sub> =CH <sub>2</sub> 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
<b>O + CF<sub>2</sub>-CFCF-CF<sub>2</sub> → products</b>							
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 <sub>ref</sub> from products in competing expts.							
Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products							
O from Hg-photosensitized decompn. of N <sub>2</sub> O.							
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(<sup>3</sup>P) Reactions with Haloalkenes and Ketenes -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + CH <sub>2</sub> =CHCH <sub>2</sub> Cl → products Oxygen atom + 1-Propene, 3-chloro-	EX	299±4	(6.14±0.36)(11)				2
84 PAR/SAW1  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 <sub>3</sub> C(CF <sub>3</sub> )=CH <sub>2</sub> → products Oxygen atom + 1-Propene, 2-trifluoromethyl-	RL	296	0.077			2/2	
68 MOS/JEN  k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + 1-Butene → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. Normalized absolute k=1.7(11) (73 HER/HUI). For updated normalized k see 86 CVE.							
71 MOS  k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. Normalized absolute k=2.6(11) (73 HER/HUI). For updated normalized k see 86 CVE.	RL	296	0.55			2/2	
73 HER/HUI	SE	296	2.0(11)			2	1.4
74 JON/MOS  k/k <sub>ref</sub> from products in competing expts.: 298K: 0.552; 423K: 0.637. Ref. Rn: O + CH <sub>2</sub> =CH <sub>2</sub> → products O from Hg-photosensitized decompr. of N <sub>2</sub> O. Current normalized values (86 CVE): k(298)=2.43(11), A=5.82(12), B=942	RL	298-423	0.909	142		2/2	
86 CVE  Derived from relative k (68 MOS/JEN) using for 1-Butene k=2.50(12).	RN	296	1.03(11)			2	
Derived from relative k (71 MOS) using for Ethylene k=4.4(11).	RN	296	2.42(11)			2	
Derived from relative k (74 JON/MOS) using for Ethylene k=4.4(11).	RN	298	2.43(11)			2	
Derived from relative k's (74 JON/MOS) using for Ethylene A=6.40(12), B=800.	RN	298-423	5.82(12)	942		2	
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(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>2</sub>FCH<sub>2</sub>CH=CH<sub>2</sub> → products</b>							
Oxygen atom + 1-Butene, 4-fluoro-							
69 MOS/JEN	RL	296	0.575			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + 1-Butene → products							
O from Hg-photosensitized decomn. of N <sub>2</sub> O. 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
<b>O + CH<sub>3</sub>CH<sub>2</sub>CF=CF<sub>2</sub> → products</b>							
Oxygen atom + 1-Butene, 1,1,2-trifluoro-							
69 MOS/JEN	RL	296	1.00			2/2	
k/k <sub>ref</sub> from products in competing expts.: Ref. Rn: O + 1-Propene → products							
O from Hg-photosensitized decomn. of N <sub>2</sub> O. 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 <sub>ref</sub> from products in competing expts.: Ref. Rn: O + CH <sub>3</sub> C(CF <sub>3</sub> )=CH <sub>2</sub> → products							
O from Hg-photosensitized decomn. of N <sub>2</sub> O. 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 <sub>3</sub> C(CF <sub>3</sub> )=CH <sub>2</sub> k=2.26(11).							
Recommended value of k	RE	298	(2.45±0.05)(12)			2	1.2
<b>O + CH<sub>2</sub>=CO → adduct(EXV)</b>							
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(<sup>3</sup>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	k err. units factor
<b>O + CH<sub>2</sub>=CO → adduct(EXV) -- Continued</b>							
73 JON/BAY	EX	296±2	(1.7±0.4)(11)				2
Flow system with 0.5-4 torr N <sub>2</sub> as principal flow gas. Photoionizn. mass spec. analysis.							
O atoms from N + NO → N <sub>2</sub> + 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
<b>O + CH<sub>3</sub>CH=CO → adduct(EXV)</b>							
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
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH=CO → adduct(EXV)</b>							
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(<sup>3</sup>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	k err. units factor
<b>O + (CH<sub>3</sub>)<sub>2</sub>C=CO → adduct(EXV)</b>							
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±0.5)(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(<sup>3</sup>P) 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 factor
<b>O + CH=CH → products</b>						
Oxygen atom + Ethyne (Acetylene)						
Main rn. products are: CO + CH <sub>2</sub> 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 <sub>2</sub> .						
k derived from rates of product formation.						
66 SAU/HEI	RL 297-398		*)		1310	2/2
*) k/k <sub>ref</sub> from products in competing expts:						
0.193(297K), 0.296(343K), 0.566(398K)						
Ref. Rn: O + CF <sub>2</sub> =CF <sub>2</sub> → products						
O from Hg-photosensitized decomprn. of N <sub>2</sub> O.						
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 <sub>2</sub> 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
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 <sub>2</sub> in He.						

Table 4.3. Data for O(<sup>3</sup>P) 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 k err. units factor
<b>O + CH=CH → products -- Continued</b>						
68 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 <sub>2</sub> as principal flow gas. Photoionizn. mass spec. analysis. O atoms from N + NO → N <sub>2</sub> + O	EX 296±2		(9.7±1.5)(10)			2
73 HER/HUI Study of CH=CH/O <sub>2</sub> flame front structure. Molecular beam sampling coupled with mass spectrometer. k(298K)=7.8(10) (calcd. from Arrh. Eq.).	SE 298 SE 1000 SE 200-700		9.5(10) 8.3(12) 1.4(13)		1500	2 1.1 1.4 1.2
77 VAN/VAN 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 <sub>2</sub> + 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(<sup>3</sup>P) 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
<b>O + CH≡CH → CO + CH<sub>2</sub></b>							
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 <sub>2</sub> O decomposition. Atomic Resonance 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							
<b>O + CH≡CH → H + CH=C=O</b>							
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 <sub>2</sub> O decomposition. Atomic-resonance-absorption-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(<sup>3</sup>P) 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	k err. units factor
<b>O + CD≡CD → products</b>							
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
<b>O + CH<sub>3</sub>C≡CH → products</b>							
Oxygen atom + 1-Propyne (Methylacetylene)							
Main reaction channel at lower T is:							
O + CH <sub>3</sub> C≡CH → CO + CH <sub>3</sub> CH:							
67 BRO/THR	EX	298	(4±1)(11)			2	
Fast-flow reactor. ESR. N <sub>2</sub> 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 <sub>2</sub> 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(298K)=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 <sub>2</sub> + 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(<sup>3</sup>P) 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
<b>O + CH<sub>3</sub>C≡CH → H + [C<sub>3</sub>H<sub>3</sub>O]<sup>·</sup></b>							
A path in the Rn. O + CH <sub>3</sub> C≡CH → products							
81 ALE/DUB 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.).	EX	295-545	(3.6±1.2)(12)		1320±220	2	
Recommended upper limit value of k Provisional recommendation.	RE	298	≤ 4.3(10)			2	1.2
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
<b>O + CH≡C≡CH → products</b>							
Oxygen atom + 1,3-Butadiyne (Diacetylene)							
66 NIK/WEI Discharge-flow system. Mass spectrometer,	EX	300	(3.98±0.48)(11)			2	
67 NIK Fast flow system-Time of flight mass spectr. O from N+NO rn.	EX	300	(9.0±1.2)(11)			2	
73 JON/BAY Flow system with 0.5-4 torr N <sub>2</sub> as principal flow gas. Photoionizn. mass spec. analysis. O atoms from N + NO → N <sub>2</sub> + O Rn.	EX	296±2	(1.6±0.5)(12)			2	
73 HER/HUI	SE	300	9(11)			2	1.4
75 HOM/SCH k(298K)=1.3(12) (calcd. from Arrh. Eq.). Isothermal low pressure flow system. Quadrupole mass spectrometer. O from microwave discharge in O <sub>2</sub> /He mixtures or from N+NO rn.	EX	297-343	8.0(13)		1230	2	
81 WEL k(298K)=1.5(12) (calcd. from Arrh. Eq.). Discharge flow system. Mass spec. analysis.	EX	295-1000	2.7(13)		866	2	
83 HOM/WEL 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 → N <sub>2</sub> + O Rn.	EX	300-1300	(2.8±0.5)(13)		870±80	2	
84 WAR k(298K)=1.5(12) (calcd. from Arrh. Eq.).	SE	300-1000	2.7(13)		866	2	
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(<sup>3</sup>P) 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.
<b>O + CH<sub>2</sub>=CHC≡CH → products</b>							
Oxygen atom + 1-Butene-3-yne (Vinylacetylene)							
83 HOM/WEL 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 <sub>2</sub> + O Rn.	EX	300-1300	(3.0±1.1)(13)	910±100	2		
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
<b>O + CH<sub>3</sub>CH<sub>2</sub>C≡CH → CO + CH<sub>3</sub>CH=CH<sub>2</sub></b>							
Oxygen atom + 1-Butyne (Ethylacetylene)							
75 HER/WAG1 k(298K)=1.2(12) (calcd. from Arrh. Eq.). Isothermal flow system. P=5 torr. Carrier gas He. O from microwave discharge in O <sub>2</sub> or NO, monitored by time-of-flight mass spectromtr.	EX	290-357	1.7(13)	800	2		
77 UMS/LIN NO <sub>2</sub> Flash-photolysis-CO laser resonant absorption. Ref. rn.: O+propyne → products. k/k(ref) from computer modeling of CO formmn. rates, normalized by taking k(ref)=4.2(11).	RN	298	5.0(11)			2	
83 HOM/WEL 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 <sub>2</sub> + O Rn.	EX	300-1300	(2.3±0.7)(13)	870±80	2		
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
<b>O + CH<sub>3</sub>C≡CCH<sub>3</sub> → CO + CH<sub>3</sub>CH=CH<sub>2</sub></b>							
Oxygen atom + 2-Butyne (Dimethylacetylene)							
75 HER/WAG2 Estimated error limits approx. ±25%. Isothermal flow system. P=5 torr. Carrier gas He. O from microwave discharge in O <sub>2</sub> or NO, monitored by time-of-flight mass spectromtr.	EX	298	2.9(12)			2	
	EX	290-360	6(13)	900	2		

Table 4.3. Data for O(<sup>3</sup>P) 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
<b>O + CH<sub>3</sub>C≡CH → CO + CH<sub>3</sub>CH=CH<sub>2</sub> -- Continued</b>							
77 UMS/LIN	RN	298	1.6(12)				2
NO <sub>2</sub> 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).							
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
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>C≡CH → CO(EXV) + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH:</b> Oxygen atom + 1-Pentyne (n-Propylacetylene)							
80 SHA/BUR	RN	300	(4.9±0.6)(11)				2
NO <sub>2</sub> 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).							
Recommended value of k (80 SHA/BUR value using k(ref)=8.6(10)). Provisional recommendation.	RE	298	4.5(11)				2 1.5
<b>O + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>C≡CH → CO(EXV) + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH:</b> Oxygen atom + 1-Hexyne (n-Butylacetylene)							
80 SHA/BUR	RN	300	(3.6±0.4)(11)				2
NO <sub>2</sub> 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).							
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(<sup>3</sup>P) 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
<b>O + C<sub>6</sub>H<sub>6</sub> → products</b>							
Oxygen atom + Benzene							
61 BOO/CVE	RL	393-494	1.04			1993	2/2
k/k <sub>ref</sub> from products in competing expts.: 393K: 6.55(-3); 494K: 1.84(-2).							
k <sub>ref</sub> : 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 <sub>2</sub> or N <sub>2</sub> O. 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 <sub>2</sub> in He)-Mass spec- trometer. k(298K): (2.8±0.70)(10). (Same k's obtained using O from N+NO rxn.)							
73 HER/HUI	SE	298	2.4(10)			2	2
	SE	250-500	2.0(13)			2000	2
74 ATK/PIT2	EX	300	(1.44±0.2)(10)			2	
Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N <sub>2</sub> O. 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 <sub>2</sub> O. 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 <sub>2</sub> and NO. Quoted errors are estimated overall limits.							
82 NIC/GUMI	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 <sub>2</sub> . 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

Table 4.4. Data for O(<sup>3</sup>P) Reactions with Aromatic Hydrocarbons -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, E-B(ref)	k,A	k err. units factor
<b>O + C<sub>6</sub>D<sub>6</sub> → products</b>							
Oxygen atom + Benzene-d <sub>6</sub>							
72 BON/KIM	RL	298	1.03±0.02			2/2	
Ref. Rn.: O + C <sub>6</sub> H <sub>6</sub> → products							
k/k <sub>ref</sub> : 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 <sub>2</sub> .							
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 <sub>6</sub> H <sub>6</sub>							
<b>O + C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> → products</b>							
Oxygen atom + Benzene, methyl-							
61 JON/CVE	RL	393-495	1.02		1600	2/2	
k/k <sub>ref</sub> from products in competing expts.							
393.4K: 1.74(-2); 495.3K: 4.02(-2).							
k <sub>ref</sub> : 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 <sub>2</sub> or N <sub>2</sub> O. k from absorption tracings							
of (not positively identified) transients.							
70 GRO/MOS	RL	303	4.37			2/2	
k/k <sub>ref</sub> : 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 <sub>2</sub> O.							
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(<sup>3</sup>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
<b>O + C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> → products -- Continued</b>							
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 <sub>2</sub> O.							
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 <sub>2</sub> 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 <sub>2</sub> . 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
 <b>O + C<sub>6</sub>H<sub>5</sub>CD<sub>3</sub> → products</b>							
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 <sub>2</sub> . 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 factor
<b><math>O + C_6H_5CH_2CH_3 \rightarrow</math> products</b>						
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 <sub>ref</sub> : 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
 <b><math>O + o-CH_3C_6H_4CH_3 \rightarrow</math> products</b>						
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 <sub>ref</sub> : 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/PITZ	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
Flash photolysis-Resonance fluorescence. O from vac. uv photol. of $O_2$ . Error=2σ.						
EX 298-600 (2.35±0.51)(13)						
1540±80						

Table 4.4. Data for O(<sup>3</sup>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	k err. units factor
<b>O + o-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub> → products -- Continued</b>							
86 CVE Derived from relative k data (70 GRO/MOS). using for Benzene k(298K)=1.22(10).	RN	303	1.22(11)			2	
Recommended value of k	RE	298	1.2(11)			2	1.3
Recommended values of Arrhenius A and l	RE	298-600	(1.5±1.2)(13)	1382±300	2	2	
 <b>O + o-CD<sub>3</sub>C<sub>6</sub>D<sub>4</sub>CD<sub>3</sub> → products</b>							
Oxygen atom + o-Xylene-d10							
82 NIC/GUM2 Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O <sub>2</sub> . Error=2σ.	EX	298	(1.20±0.13)(11)			2	
	EX	298-600	(2.06±0.37)(13)	1550±70	2		
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	
 <b>O + m-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub> → products</b>							
Oxygen atom + m-Xylene							
68 MAN/SAU *)T probably ~298K. O from pulse radiolysis of CO <sub>2</sub> or N <sub>2</sub> O. k from absorption tracings of (not positively identified) transients.	EX	*)	(7.7±2.0)(11)			2	
70 GRO/MOS k/k <sub>ref</sub> : 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)	RL	303	23.0			2/2	
73 HER/HUI	SE	298	7.7(11)			2	2
74 ATK/PIT2 Phase shift-O+NO chemiluminescence. O from Hg-photosensitized decomp. of N <sub>2</sub> O. Quoted errors are estimated overall limits.	EX	299	(2.12±0.21)(11)			2	
75 ATK/PIT (See Notes in preceding entry, 74 ATK/PIT2)	EX	299-392	7.7(12)	1082±150	2		
82 NIC/GUM2 Flash photolysis-Resonance fluorescence. O from vac. uv photol. of O <sub>2</sub> . Error=2σ.	EX	298	(2.37±0.26)(11)			2	
	EX	298-600	(2.28±0.51)(13)	1350±90	2		
86 CVE Derived from relative k data (70 GRO/MOS) using for Benzene k(298K)=1.22(10).	RN	303	2.81(11)			2	

Table 4.4. Data for O(<sup>3</sup>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 factor	k err.
<b>O + m-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub> → products -- Continued</b>							
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	
<b>O + m-CD<sub>3</sub>C<sub>6</sub>D<sub>4</sub>CD<sub>3</sub> → products</b>							
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 <sub>2</sub> . 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	
<b>O + p-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub> → products</b>							
Oxygen atom + p-Xylene							
68 MAN/SAU	EX	*	(4.5±1.4)(11)			2	
*)T probably ~298K. O from pulse radiolysis of CO <sub>2</sub> or N <sub>2</sub> O. k from absorption tracings of (not positively identified) transients.							
70 GRO/MOS	RL	303	9.77			2/2	
k/k <sub>ref</sub> : 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-photo sensitized decomp. of N <sub>2</sub> O.							
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 <sub>2</sub> . 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(<sup>3</sup>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 factor	k'err
<b>O + C<sub>6</sub>H<sub>5</sub>C(CH<sub>3</sub>)<sub>3</sub> → products</b>							
Oxygen atom + Benzene, t-butyl-							
70 GRO/MOS	RL	303	3.60				2/2
k/k <sub>ref</sub> : 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.							
<b>O + 1,2,3-(CH<sub>3</sub>)<sub>3</sub>C<sub>6</sub>H<sub>3</sub> → products</b>							
Oxygen atom + Benzene, 1,2,3-trimethyl-							
70 GRO/MOS	RL	303	25.0				2/2
k/k <sub>ref</sub> : 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 <sub>2</sub> O. 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
<b>O + 1,2,4-(CH<sub>3</sub>)<sub>3</sub>C<sub>6</sub>H<sub>3</sub> → products</b>							
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 <sub>2</sub> O. Quoted errors are estimated overall limits.							
75 ATK/PIT	EX	299-392	8.35(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(<sup>3</sup>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	k err. units factor
<b>O + 1,3,5-(CH<sub>3</sub>)<sub>3</sub>C<sub>6</sub>H<sub>3</sub> → products</b>							
Oxygen atom + Benzene, 1,3,5-trimethyl-							
70 GRO/MOS	RL	303	80.0				2/2
k/k <sub>ref</sub> : 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 <sub>2</sub> O.							
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
 <b>O + C<sub>5</sub>H<sub>5</sub>N → products</b>							
Oxygen atom + Pyridine							
68 MAN/SAU	EX	*)	(1.0±0.3)(11)				2
*)T probably ~298K. O from pulse radiolysis of CO <sub>2</sub> or N <sub>2</sub> O. 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 <sub>2</sub> O) 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	2.0(12)			1260±300	2 2
Provisional recommendation.							

Table 4.4. Data for O(<sup>3</sup>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 factor	k err.
<b>O + C<sub>6</sub>H<sub>5</sub>Cl → products</b>							
Oxygen atom + Benzene, chloro-							
68 MAN/SAU	EX *)		(3.1±0.8)(11)				2
			*)T probably ~298K. O from pulse radiolysis of CO <sub>2</sub> or N <sub>2</sub> O. k from absorption tracings of (not positively identified) transients.				
Recommended value of k	RE	298	3(11)				2 3
Provisional recommendation.							
<b>O + C<sub>6</sub>H<sub>5</sub>F → products</b>							
Oxygen atom + Benzene, fluoro-							
68 MAN/SAU	EX *)		(2.7±0.6)(10)				2
			*)T probably ~298K. O from pulse radiolysis of CO <sub>2</sub> or N <sub>2</sub> O. k from absorption tracings of (not positively identified) transients.				
70 GRO/MOS	RL	303	0.67				2/2
			k/k <sub>ref</sub> : 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.							
<b>O + C<sub>6</sub>H<sub>5</sub>CF<sub>3</sub> → products</b>							
Oxygen atom + Benzene, trifluoromethyl-							
70 GRO/MOS	RL	303	0.20				2/2
			k/k <sub>ref</sub> : 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.							

## 5. References to the Data Tables

- 57 BEN/AXW Benson, S. W., and Axworthy, A. E., Jr., "Mechanism of the Gas Phase, Thermal Decomposition of Ozone," *J. Chem. Phys.* **26**, 1718 (1957).
- 57 FOR/END Ford, H. W., and Endow, N., "Rate Constants at Low Concentrations. IV. Reactions of Atomic Oxygen with Various Hydrocarbons," *J. Chem. Phys.* **27**, 1277 (1957).
- 58 KAU Kaufman, F., "Air Afterglow and Kinetics of Some Reactions of Atomic Oxygen," *J. Chem. Phys.* **28**, 352 (1958).
- 59 CVE Cvetanović, R. J., "Relative Rates of Reactions of Oxygen Atoms with Olefins," *J. Chem. Phys.* **30**, 19 (1959).
- 60 CVE1 Cvetanović, R. J., "Electrophilic Character of Oxygen Atoms," *Can. J. Chem.* **38**, 1678 (1960).
- 60 CVE2 Cvetanović, R. J., "Temperature Dependence of the Rates of Addition of Oxygen Atoms to Olefins," *J. Chem. Phys.* **33**, 1063 (1960).
- 60 CVE/DOY Cvetanović, R. J., and Doyle, L. C., "Reaction of Oxygen Atoms with Butadiene," *Can. J. Chem.* **38**, 2187 (1960).
- 60 ELI/SCH Elias, L., and Schiff, H. I., "Absolute Rate Measurements of O-Atom Reactions with Ethylene and with Butane," *Can. J. Chem.* **38**, 1657 (1960).
- 61 BOO/CVE Boocock, G., and Cvetanović, R. J., "Reaction of Oxygen Atoms with Benzene," *Can. J. Chem.* **39**, 2436 (1961).
- 61 JON/CVE Jones, G. R. H., and Cvetanović, R. J., "Reaction of Oxygen Atoms with Toluene," *Can. J. Chem.* **39**, 2444 (1961).
- 63 AVR/KOL Avramenko, L. I., Kolesnikova, R. V., and Savinova, G. I., "Rate Constants and Mechanism of Reaction of Oxygen Atoms with Ethylene, Propylene and Isobutylene," *Bull. Acad. Sci. USSR, Div. Chem. Sci.* **30** (1973); tr. of *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk* **36** (1963).
- 63 AZA/NAL Azatyan, V. V., Nalbandyan, A. B., and Mengyuan, T., "Determination of the Rate Constants of the Elementary Reactions of Atomic Hydrogen and Oxygen with Ethylene," *Dokl. Phys. Chem. (Engl. Transl.)* **149**, 312 (1963); tr. of *Dokl. Akad. Nauk SSSR* **149**, 1095 (1963).
- 63 ELI Elias, L., "Reinvestigation of Some Absolute Rate Measurements of O-atom Reactions with Olefins," *J. Chem. Phys.* **38**, 989 (1963).
- 64 AVR/KOL Avramenko, L. I., and Kolesnikova, R. V., "Mechanism and Rate Constants of Elementary Gas Phase Reactions Involving Hydroxyl and Oxygen Atoms," *Adv. Photochem.* **2**, 25 (1964).
- 65 ARR/BRE1 Arrington, C. A., Brennen, W., Glass, G. P., Michael, J. V., and Niki, H., "Comments," on A. Fontijn, et al., "Chemi-Ionization and Chemi-luminescence in the Reaction of Atomic Oxygen with  $C_2H_2$ ,  $C_2D_2$  and  $C_2H_4$ ," *Symp. Combust.* **10**, (Combustion Institute, Pittsburgh, 1965) 557.
- 65 ARR/BRE2 Arrington, C. A., Brennen, W., Glass, G. P., Michael, J. V., and Niki, H., "Reactions of Atomic Oxygen with Acetylene. I. Kinetics and Mechanisms," *J. Chem. Phys.* **43**, 525 (1965).
- 65 AVR/KOL Avramenko, L. I., Kolesnikova, R. B., and Savinova, G. I., "Mechanism and Rate Constant for the Reaction of Oxygen Atoms with Acetylene," *Bull. Acad. Sci. USSR, Div. Chem. Sci.* **396** (1965); tr. of *Izv. Akad. Nauk SSSR, Ser. Khim.* **408** (1965).
- 65 SAU/HEI1 Saunders, D., and Heicklen, J., "The Reaction of Oxygen Atoms with Tetrafluoroethylene," *J. Am. Chem. Soc.* **87**, 2088 (1965).
- 65 SAU/HEI2 Saunders, D., and Heicklen, J., "The Reaction of Oxygen Atoms with Perfluoropropene," *J. Am. Chem. Soc.* **87**, 4062 (1965).
- 65 SUL/WAR Sullivan, J. O., and Warneck, P., "Rate Constant for the Reaction of Oxygen Atoms with Acetylene," *J. Phys. Chem.* **69**, 1749 (1965).
- 66 NIK/WEI Niki, H., and Weinstock, B., "Reaction of  $O(^3P)$  Atoms with Diacetylene," *J. Chem. Phys.* **45**, 3468 (1966).
- 66 SAU/HEI Saunders, D., and Heicklen, J., "Some Reactions of Oxygen Atoms. I.  $C_2F_4$ ,  $C_3F_6$ ,  $C_2H_2$ ,  $C_2H_4$ ,  $C_3H_6$ ,  $1-C_4H_8$ ,  $C_2H_6$ ,  $c-C_3H_8$ , and  $C_3H_8$ ," *J. Phys. Chem.* **70**, 1950 (1966).
- 67 BRO/THR Brown, J. M., and Thrush, B. A., "E.S.R. Studies of the Reactions of Atomic Oxygen and Hydrogen with Simple Hydrocarbons," *Trans. Faraday Soc.* **63**, 630 (1967).
- 67 NIK Niki, H., "Erratum: Reactions of  $O(^3P)$  Atoms with Formaldehyde and Diacetylene," *J. Chem. Phys.* **47**, 3102 (1967).
- 67 TAN/TSU Tanaka, C., Tsuchiya, S., and Hikida, T., "Reaction of Oxygen Atoms with Ethylene," *J. Fac. Eng., Univ. Tokyo, Ser. A* **5**, 62 (1967).
- 68 CAR/GAY Carr, R. W., Jr., Gay, I. D., Glass, G. P., and Niki, H., "Reaction of Ketene with Atomic Hydrogen and Oxygen," *J. Phys. Chem.* **49**, 846 (1968).
- 68 MAN/SAU Mani, I., and Sauer, M. C., Jr., "A Pulsed-Radiolysis Study of the Gas-Phase Reaction of Oxygen Atoms with Benzene and Related Compounds: Rate Constants and Transient Spectra," in 'Radiation Chemistry. Advances in Chemistry Series 82', p. 142 (1968).
- 68 MOS/JEN Moss, S. J., and Jennings, K. R., "Reaction of Oxygen Atoms with 2-(Trifluoromethyl)-Propene," *Trans. Faraday Soc.* **64**, 686 (1968).
- 69 BRA/TSE Bradley, J. N., and Tse, R. S., "Electron Spin Resonance Study of the Reaction between Oxygen Atoms and Acetylene," *Trans. Faraday Soc.* **65**, 2685 (1969).
- 69 HOY/WAG Hoyermann, K., Wagner, H. G., and Wolfram, J., "Zur Reaktion  $O + C_2H_2 \rightarrow CO + CH_2$ ," *Z. Phys. Chem. N.F.* **63**, 193 (1969).
- 69 JAM/GLA James, G. S., and Glass, G. P., "Some Aspects of Acetylene Oxidation," *J. Chem. Phys.* **50**, 2268 (1969).
- 69 MOS/JEN Moss, S. J., and Jennings, K. R., "Relative Rate Constants for the Reaction of Ground-State Oxygen Atoms with Partly Fluorinated Propylenes and Butenes," *Trans. Faraday Soc.* **65**, 415 (1969).
- 69 NIK/DAB Niki, H., Daly, E. E., and Weinstock, B., "Mass Spectrometric Study of the Kinetics and Mechanism of the Ethylene-Atomic Oxygen Reaction by the Discharge-Flow Technique at 300 K," *Symp. Combust.* **12** (Combustion Institute, Pittsburgh, 1969) 277.
- 69 TYE Tyerman, W. J. R., "Rate Parameters for Reaction of Oxygen Atoms with  $C_2F_4$ ,  $CF_2CFCI$ ," and  $CF_2CCl_2$ ," *Trans. Faraday Soc.* **65**, 163 (1969).
- 69 WES/DEHI Westenberg, A. A., and de Haas, N., "Absolute Measurements of the  $O + C_2H_2$  Rate Coefficient," *J. Phys. Chem.* **73**, 1181 (1969).
- 69 WES/DEH2 Westenberg, A. A., and de Haas, N., "Absolute Measurements of the  $O + C_2H_4$  Rate Coefficient," *Symp. Combust.* **12** (Combustion Institute, Pittsburgh, 1969) 289.
- 70 GRO/MOS Grovenstein, E., Jr., and Mosher, A. J., "Reaction of Atomic Oxygen with Aromatic Hydrocarbons," *J. Am. Chem. Soc.* **92**, 3810 (1970).
- 71 ATK/CVE Atkinson, R., and Cvetanović, R. J., "Determination of the Absolute Values of the Rate Constants of the Reactions of  $O(^3P)$  Atoms with Alkenes by a Modulation Technique," *J. Chem. Phys.* **55**, 639 (1971).

- 71 HUI/HER Huie, R. E., Herron, J. T., and Davis, D. D., "Absolute Rate Constants for the Reaction of Atomic Oxygen with 1-Butene over the Temperature Range of 259–493 °K," *J. Phys. Chem.* **75**, 3902 (1971).
- 71 MOS Moss, S. J., "Relative Rate Constants for the Reaction of Ground-state Oxygen Atoms with Fluorinated Ethylenes," *Trans. Faraday Soc.* **67**, 3503 (1971).
- 71 STO/HEI Stockburger, L., III, and Heicklen, J., "Reaction of Oxygen Atoms with 1,3-Perfluorobutadiene," *J. Am. Chem. Soc.* **93**, 3333 (1971).
- 71 STU/NIK Stuhl, F., and Niki, H., "Determination of Rate Constants for Reactions of O Atoms with  $C_2H_2$ ,  $C_2D_2$ ,  $C_2H_4$ , and  $C_3H_6$  Using a Pulsed Vacuum-uv Photolysis-Chemiluminescent Method," *J. Chem. Phys.* **55**, 3954 (1971).
- 72 ATK/CVE Atkinson, R., and Cvjetanović, R. J., "Activation Energies of the Addition of  $O(^3P)$  Atoms to Olefins," *J. Chem. Phys.* **56**, 432 (1972).
- 72 BON/KIM Bonanno, R. A., Kim, P., Lee, J.-H., and Timmons, R. B., "Kinetics of the Reaction of  $O(^3P)$  Atoms with Benzene," *J. Chem. Phys.* **52**, 1377 (1972).
- 72 DAV/HUI Davis, D. D., Huie, R. E., Herron, J. T., Kurylo, M. J., and Braun, W., "Absolute Rate Constants for the Reaction of Atomic Oxygen with Ethylene over the Temperature Range 232–500 °K," *J. Chem. Phys.* **56**, 4868 (1972).
- 72 HUI/HER1 Huie, R. E., Herron, J. T., and Davis, D. D., "Absolute Rate Constants for the Addition and Abstraction Reactions of Atomic Oxygen with 1-Butene over the Temperature Range 190–491 K," *J. Phys. Chem.* **76**, 3311 (1972).
- 72 HUI/HER2 Huie, R. E., Herron, J. T., and Davis, D. D., "Rates of Reaction of Atomic Oxygen with  $C_2H_3F$ ,  $C_2H_3Cl$ ,  $C_2H_3Br$ , 1,1- $C_2H_2F_2$ , and 1,2- $C_2H_2F_2$ ," *Int. J. Chem. Kinet.* **4**, 521 (1972).
- 72 KUR Kurylo, M. J., "Absolute Rate Constants for the Addition of  $O(^3P)$  Atoms to Propylene," *Chem. Phys. Lett.* **14**, 117 (1972).
- 72 STU/NIK Stuhl, F., and Niki, H., "Absolute Rate Constants for the Reactions of  $O(^3P)$  Atoms with  $C_2H_4$  and  $C_2D_4$ ," *J. Chem. Phys.* **57**, 5403 (1972).
- 73 DAV/HUI Davis, D. D., Huie, R. E., and Herron, J. T., "Direct Rate Measurements Showing Negative Temperature Dependence for Reaction of Atomic Oxygen with cis-2-butene and Tetramethylethylene," *J. Chem. Phys.* **59**, 628 (1973).
- 73 HER/HUI Herron, J. T., and Huie, R. E., "Rate Constants for the Reactions of Atomic Oxygen ( $O(^3P)$ ) with Organic Compounds in the Gas Phase," *J. Phys. Chem. Ref. Data* **2**, 467 (1973).
- 73 JON/BAY Jones, I. T. N., and Bayes, K. D., "The Kinetics and Mechanism of the Reaction of Atomic Oxygen with Acetylene," *Proc. R. Soc. Lond. A* **335**, 547 (1973).
- 73 KUR/HUI Kurylo, M. J., and Huie, R. E., "Flash Photolysis Resonance Fluorescence Study of the Addition of  $O(^3P)$  Atoms to  $C_2H_4$  and  $C_2D_4$  at 298 °K," *J. Chem. Phys.* **58**, 1258 (1973).
- 73 PEE/MAH Peeters, J., and Mahnen, G., "Structure of Ethylene - Oxygen Flames. Reaction Mechanism and Rate Constants of Elementary Reactions," *Combust. Inst., European Symp.* 1973, edited by F. J. Weinberg (Academic Press, New York) 53.
- 74 ATK/PIT1 Atkinson, R., and Pitts, J. N., Jr., "Temperature Dependence of the Reaction Rate Constants for  $O(^3P)$  Atoms with  $C_2H_4$ ,  $C_3H_6$  and  $NO(M = N_2O)$ , Determined by a Modulation Technique," *Chem. Phys. Lett.* **27**, 467 (1974).
- 74 ATK/PIT2 Atkinson, R., and Pitts, J. N., Jr., "Absolute Rate Constants for the Reaction of  $O(^3P)$  Atoms with Selected Alkanes, Alkenes, and Aromatics as Determined by a Modulation Technique," *J. Phys. Chem.* **78**, 1780 (1974).
- 74 FUR/ATK Furuyama, S., Atkinson, R., Colussi, A. J., and Cvjetanović, R. J., "Determination by the Phase Shift Method of the Absolute Rate Constants of Reactions of  $O(^3P)$  Atoms with Olefins at 25 °C," *Int. J. Chem. Kinet.* **6**, 741 (1974).
- 74 HER/WAG Herbrechtsmeier, P., and Wagner, H. Gg., "Reaktion von  $O(^3P)$ -Atomen mit Methylacetylen," *Z. Phys. Chem. N. F.* **93**, 143 (1974).
- 74 JON/MOS Jones, D. S., and Moss, S. J., "Arrhenius Parameters for Reactions of Oxygen Atoms with the Fluorinated Ethylenes," *Int. J. Chem. Kinet.* **6**, 443 (1974).
- 74 MAC/THR Mack, G. P. R., and Thrush, B. A., "Reaction of Oxygen Atoms with Carbonyl Compounds. Part 3. Ketene," *J. Chem. Soc. Faraday Trans. I* **70**, 187 (1974).
- 74 MCC McCleny, W. A., "Determination of Relative Rates for Oxygen Atom-Hydrocarbon Reactions by Reduction of Oxygen Atom, Nitric Oxide Chemiluminescence," *J. Chem. Phys.* **60**, 793 (1974).
- 74 SAN/HEI Sanhueza, E., and Heicklen, J., "The Reaction of  $O(^3P)$  with  $C_2HCl_3$ ," *Int. J. Chem. Kinet.* **6**, 553 (1974).
- 74 SLA/PRU Slagle, I. R., Pruss, F. J., Jr., and Gutman, D., "Kinetics into the Steady State. I. Study of the Reaction of Oxygen Atoms with Methyl Radicals," *Int. J. Chem. Kinet.* **6**, 111 (1974).
- 75 ARR/COX Arrington, C. A., Jr., and Cox, D. J., "Arrhenius Parameters for the Reaction of Oxygen Atoms,  $O(^3P)$ , with Propyne," *J. Phys. Chem.* **79**, 2584 (1975).
- 75 ATK/PIT Atkinson, R., and Pitts, J. N., Jr., "Temperature Dependence of the Absolute Rate Constants for the Reaction of  $O(^3P)$  Atoms with a Series of Aromatic Hydrocarbons over the Range 299–392 °K," *J. Phys. Chem.* **79**, 295 (1975).
- 75 COL/SIN Colussi, A. J., Singleton, D. L., Irwin, R. S., and Cvjetanović, R. J., "Absolute Rates of Oxygen( $^3P$ ) Atom Reactions with Benzene and Toluene," *J. Phys. Chem.* **79**, 1900 (1975).
- 75 FUR/EBA Furuyama, S., and Ebara, N., "A Kinetic Study of the Reaction of  $O(^3P)$  with Toluene," *Int. J. Chem. Kinet.* **7**, 689 (1975).
- 75 GAF/ATK1 Gaffney, J. S., Atkinson, R., and Pitts, J. N., Jr., "Relative Rate Constants for the Reaction of  $O(^3P)$  Atoms with Selected Olefins, Monoterpenes, and Unsaturated Aldehydes," *J. Am. Chem. Soc.* **97**, 5049 (1975).
- 75 GAF/ATK2 Gaffney, J. S., Atkinson, R., and Pitts, J. N., Jr., "Temperature Dependence of the Relative Rate Constants for the Reaction of  $O(^3P)$  Atoms with Selected Olefins, Monoterpenes, and Unsaturated Aldehydes," *J. Am. Chem. Soc.* **97**, 6481 (1975).
- 75 GER/MOI Gershenson, Yu. M., Moin, F. B., and Yurkevich, Ya. P., "Diffusion Cloud Analog Method for the Study of Reaction Kinetics. Reaction of Atomic Oxygen with  $C_2H_2$  and  $C_2F_4$ ," *Kinet. Catal.* **16**, 1192 (1975); tr. of *Kinet. Katal.* **16**, 1373 (1975) (Russ.).
- 75 HER/WAG1 Herbrechtsmeier, P., and Wagner, H. Gg., "Reaktion von  $O(^3P)$ -Atomen mit Äthylacetylen," *Ber. Bunsenges. Phys. Chem.* **79**, 461 (1975).
- 75 HER/WAG2 Herbrechtsmeier, P., and Wagner, H. Gg., "Reaktion von  $O(^3P)$ -Atomen mit Dimethylacetylen," *Ber. Bunsenges. Phys. Chem.* **79**, 673 (1975).

- 75 HOM/SCH Homann, K. H., Schwanebeck, W., and Warnatz, J., "Reaktionen des Butadiins. II. Die Reaktion mit Sauerstoffatomen," Ber. Bunsengesell. Phys. Chem. **79**, 536 (1975).
- 75 SAN/HEI Sanhueza, E., and Heicklen, J., "The Reaction of O(<sup>3</sup>P) with CCl<sub>2</sub>CH<sub>2</sub>," J. Photochem. **4**, 1 (1975).
- 75 SIN/FUR Singleton, D. L., Furuyama, S., Cvetanović, R. J., and Irwin, R. S., "Temperature Dependence of the Rate Constants for the Reactions O(<sup>3</sup>P) + 2,3-dimethyl-2-butene and O(<sup>3</sup>P) + NO + M Determined by a Phase Shift Technique," J. Chem. Phys. **63**, 1003 (1975).
- 75 SLA/GUT Slagle, I. R., Gutman, D., and Gilbert, J. R., "Direct Identification of Products and Measurement of Branching Ratios for the Reactions of Oxygen Atoms with Vinylfluoride, Vinylchloride, and Vinylbromide," Symp. Combust. **15** (Combustion Institute, Pittsburgh, 1975) 785.
- 76 ATK/PIT Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with CH<sub>2</sub>=CHF, CH<sub>2</sub>=CHCl, and CH<sub>2</sub>=CHBr at 298 ± 2 °K," Int. J. Chem. Kinet. **8**, 475 (1976).
- 76 GIL/SLA Gilbert, J. R., Slagle, I. R., Graham, R. E., and Gutman, D., "Direct Identification of Reactive Routes and Measurement of Rate Constants in the Reactions of Oxygen Atoms with the Fluoroethylenes," J. Chem. Phys. **60**, 14 (1976).
- 76 MAN/BRA Manning, R. G., Braun, W., and Kurylo, M. J., "The Effect of Infrared Laser Excitation on Reaction Dynamics: O + C<sub>2</sub>H<sub>4</sub><sup>+</sup> and O + OCS<sup>+</sup>," J. Chem. Phys. **65**, 2609 (1976).
- 76 SIN/CVE Singleton, D. L., and Cvetanović, R. J., "Temperature Dependence of the Reactions of Oxygen Atoms with Olefins," J. Am. Chem. Soc. **98**, 6812 (1976).
- 77 ATK/PIT1 Atkinson, R., and Pitts, J. N., Jr., "Absolute Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with a Series of Olefins over the Temperature Range 298–439 °K," J. Chem. Phys. **67**, 38 (1977).
- 77 ATK/PIT2 Atkinson, R., and Pitts, J. N., Jr., "Absolute Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with Allene, 1,3-Butadiene, and Vinyl Methyl Ether over the Temperature Range 297–439 °K," J. Chem. Phys. **67**, 2492 (1977).
- 77 ATK/PIT3 Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with CH<sub>2</sub>=CHF, CH<sub>2</sub>=CHCl, and CH<sub>2</sub>=CHBr over the Temperature Range 298–442 °K," J. Chem. Phys. **67**, 2488 (1977).
- 77 MIC/LEE Michael, J. V., and Lee, J. H., "Selected Rate Constants for H, O, N, and Cl Atoms with Substrates at Room Temperatures," Chem. Phys. Lett. **51**, 303 (1977).
- 77 UMS/TIN Umstead, M. E., and Lin, M. C., "The Dynamics of CO Production from the Reaction of O(<sup>3</sup>P) with 1- and 2-Butyne," Chem. Phys. **25**, 353 (1977).
- 77 VAN/VAN Vandooren, J., and Van Tiggelen, P. J., "Reaction Mechanisms of Combustion in Low Pressure Acetylene-Oxygen Flames," Symp. Combust. **16**, (Combustion Institute, Pittsburgh, 1977) 1133.
- 77 WES/DEH Westenberg, A. A., and deHaas, N., "A Flash Photolysis-Resonance Fluorescence Study of the O + C<sub>2</sub>H<sub>2</sub> and O + C<sub>2</sub>H<sub>3</sub>Cl Reactions," J. Chem. Phys. **66**, 4900 (1977).
- 78 KOH Kohse-Höinghaus, K., Dissertation, Ruhr University, Bochum, West Germany (1978) (Quoted by 84 BRO/STU).
- 79 ATK/PIT Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with Benzene and Toluene over the Temperature Range 299–440 K," Chem. Phys. Lett. **63**, 485 (1979).
- 79 KOD Koda, S., "Mechanism of Oxygen (<sup>3</sup>P) Atom Reaction with Tetrafluoroethylene and Quenching Processes of the Emission of CF<sub>2</sub>(<sup>3</sup>B<sub>1</sub>)," J. Phys. Chem. **83**, 2065 (1979).
- 79 NIP/SIN Nip, W. S., Singleton, D. L., and Cvetanović, R. J., "Temperature Dependence of Rate Constants for Reaction of Oxygen Atoms, O(<sup>3</sup>P), with Allene and 1,3-Butadiene," Can. J. Chem. **57**, 949 (1979).
- 80 ALE/ARU Aleksandrov, E. N., Arutyunov, V. S., and Kozlov, S. N., "Study of the Reaction of Oxygen Atoms with Allene," Kinet. Katal. **21**, 1327 (1980) (Russ.).
- 80 SHA/BUR Shaub, W. M., Burks, T. L., and Lin, M. C., "Dynamics of Reactions of O(<sup>3</sup>P) Atoms with 1-Alkenes as Studied by a CO Laser Resonance Absorption Technique," Chem. Phys. **45**, 455 (1980).
- 80 SUG/ISH Sugawara, K., Ishikawa, Y., and Sato, S., "Absolute Rate Constants for the Reactions of O(<sup>3</sup>P) with Several Molecules," Bull. Chem. Soc. Jpn. **53**, 1344 (1980).
- 81 ALE/ARU Aleksandrov, E. N., Arutyunov, V. S., and Kozlov, S. N., "Investigation of the Reaction of Atomic Oxygen with Acetylene," Kinet. Catal. **22**, 391 (1981); tr. of Kinet. Katal. **22**, 513 (1981) (Russ.).
- 81 ALE/DUB Aleksandrov, E. N., Dubrovina, I. V., and Kozlov, S. N., "The Reaction of Oxygen Atoms with Methylacetylene," Kinet. Catal. **22**, 394 (1981); tr. of Kinet. Katal. **22**, 517 (1981) (Russ.).
- 81 LOH/ROT Löhr, R., and Roth, P., "Shock Tube Measurements of the Reaction Behaviour of Acetylene with O-Atoms," Ber. Bunsenges. Phys. Chem. **85**, 153 (1981).
- 81 SUG/OKA Sugawara, K., Okazaki, K., and Sato, S., "The Rate Constants of the Reactions of Hydrogen and Oxygen Atoms with Fluoroethylenes," Bull. Chem. Soc. Jpn. **54**, 358 (1981).
- 81 WEL Wellmann, C., Dissertation, T. H. Darmstadt (1981) (Quoted by 84 WAR).
- 82 BIE/HAR Biermann, H. W., Harris, G. W., and Pitts, J. N., Jr., "Photoionization Mass Spectrometer Studies of the Collisionally Stabilized Product Distribution in the Reaction of OH Radicals with Selected Alkenes at 298 K," J. Phys. Chem. **86**, 2958 (1982).
- 82 NIC/GUM1 Nicovich, J. M., Gump, C. A., and Ravishankara, A. R., "Rates of Reactions of O(<sup>3</sup>P) with Benzene and Toluene," J. Phys. Chem. **86**, 1684 (1982).
- 82 NIC/GUM2 Nicovich, J. M., Gump, C. A., and Ravishankara, A. R., "Rates of Reactions of O(<sup>3</sup>P) with Xylenes," J. Phys. Chem. **86**, 1690 (1982).
- 82 NIC/RAV Nicovich, J. M., and Ravishankara, A. R., "A Study of the Reaction of O(<sup>3</sup>P) with Ethylene," Symp. Combust. **19** (Combustion Institute, Pittsburgh, 1982) 23.
- 82 ROT/LOH Roth, P., and Löhr, R., "Direct Measurements of O-Atom Reactions with HCN and C<sub>2</sub>H<sub>2</sub> Behind Shock Waves," Proc. Intern. Symp. Shock Tubes and Waves **13**, 593 (1982).
- 82 TEM/WAG Temps, F., and Wagner, H. G., "Untersuchungen zur Produktbildung in der Reaktion von Sauerstoffatomen mit Ethylen," Max-Planck-Institut für Stoffforschung. Report No. 18 (1982) 19 pp; Chem. Abstr. **98**:215020r (1982).
- 82 WAS/TAK Washida, N., and Takagi, H., "Reaction of Cyclohexane and Cyclohexyl Radicals with Atomic and Molecular Oxygen," J. Am. Chem. Soc. **104**, 168 (1982).
- 83 FON/MAE Fonderie, V., Maes, D., and Peeters, J., "The Kinetic Coefficient of the C<sub>2</sub>H<sub>4</sub> + O Reaction over Extended Pressure and Temperature Ranges," Bull. Soc. Chim. Belg. **92**, 641 (1983).

- 83 HOM/WEL Homann, K. H., and Wellmann, Ch., "Arrhenius Parameters for the Reactions of O Atoms with Some Alkynes in the Range 300-1300 K," *Ber. Bunsen-Ges. Phys. Chem.* **87**, 527 (1983).
- 83 TAB/GON Tabarés, F. L., and González Ureña, A., "Rate Constant for the Reaction of O(<sup>3</sup>P) with Pyridine from 323 to 473 K," *J. Phys. Chem.* **87**, 4933 (1983).
- 83 WAS/HAT Washida, N., Hatakeyama, S., Takagi, H., Kyogoku, T., and Sato, S., "Reaction of Ketenes with Atomic Oxygen," *J. Chem. Phys.* **78**, 4533 (1983).
- 84 BRO/STU Browarzik, R., and Stuhl, F., "Temperature Dependence of the Rate Constants for the Reactions of Oxygen Atoms with Ethene, Propene, and 1-Butene," *J. Phys. Chem.* **88**, 6004 (1983).
- 84 CVE/SIN Cvetočić, R. J., and Singleton, D. L., "Reaction of Oxygen Atoms with Olefins," *Rev. Chem. Inter.* **5**, 183 (1984).
- 84 PAR/SAW1 Park, J.-Y., Sawyer, P. F., Heaven, M. C., and Gutman, D., "Pressure Dependence of Chemical Branching in the Oxygen-Atom Reaction with Allyl Chloride," *Chem. Phys. Lett.* **103**, 408 (1984).
- 84 PAR/SAW2 Park, J.-Y., Sawyer, P. F., Heaven, M. C., and Gutman, D., "Chemical Branching in the Oxygen-Atom Reaction with Vinyl Fluoride. Pressure Dependence of the Route O + C<sub>2</sub>H<sub>3</sub>F → CH<sub>2</sub>F + HCO," *J. Phys. Chem.* **88**, 2821 (1984).
- 84 PER1 Perry, R. A., "Absolute Rate Constants for the Reaction of O(<sup>3</sup>P) Atoms with Ethylene, Propylene, and Propylene-d<sub>6</sub> over the Temperature Range 258-861 K," *J. Chem. Phys.* **80**, 153 (1984).
- 84 PER2 Perry, R. A., "Kinetics of the Reaction of O Atoms with Olefins over Temperature Range 260-860 K using Laser Photolysis-Chemiluminescence," 188th ACS Natl. Meeting, Philadelphia, Pa., Aug. 26-31 (1984); Div. Phys. Chem., Abstr. No. 241.
- 84 WAR Warnatz, J., "Rate Coefficients in the C/H/O System," in 'Combustion Chemistry', Ed. W.C. Gardiner, Jr., Springer-Verlag, 1984, p. 197.
- 86 CVE Cvetočić, R. J., The present evaluation.
- 86 PEE/SCH Peeters, J., Schaevers, M., and Vincquier, C., "Ketenyl Radical Yield of the Elementary Reaction of Ethyne with Atomic Oxygen at T = 290-540 K," *J. Phys. Chem.* **90**, 6552 (1986).