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Rate Constants for the Decay and Reactions of the Lowest Electronically Excited Singlet State of Molecular Oxygen in Solution

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The available rate data on the reactivity and physical deactivation of molecular oxygen in its first electronic excited state ($^1\Delta_g$) in liquid solution have been critically compiled. Where possible, relative rates reported in the literature have been normalized to standard values selected by a statistical analysis of the experimental data. Second order rate constants for the deactivation and chemical reaction of singlet oxygen are reported for 670 compounds. Additionally, psuedo first order rate constants (k_d) for solvent deactivation of singlet oxygen are reported for 50 different solvents.

Key words: Chemical kinetics; data compilation; oxidation; photochemistry; rates; review; singlet oxygen; solution.

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1. Introduction

Direct and sensitized photo-oxygenations of various organic and biological substrates in fluid solution have been much studied since they were first observed at the beginning of the century [1-3][1]. Several mechanisms for photo-oxygenations have been established including that involving the lowest excited singlet state of oxygen as an oxidizing intermediate. Although singlet oxygen was proposed by Kautsky as a possible reaction intermediate in dye-sensitized photo-oxygenations as early as 1931 [4,5], it was only in 1964 that Foote and Wexler [6] and Corey and Taylor [7] respectively demonstrated that the oxygenation product distribution for several substrates, from chemically generated (using H_2O_2/NaOCl) and from radio-frequency generated, singlet oxygen, was the same as in sensitized photo-oxygenations of these same substrates. Only then was the photo-oxygenation mechanism involving singlet oxygen generally accepted.

Since then thousands of reactions of singlet oxygen have been studied some of which have found application in preparative organic chemistry [8]. Since oxygen is ubiquitous and efficiently quenches electronically excited states, singlet oxygen is likely to be formed following irradiation in countless situations, and a better understanding of the properties of singlet oxygen will help with differentiating those systems where the role of singlet oxygen is indeed crucial. Equally, further knowledge on other potentially competitive mechanisms is also necessary. There is strong evidence for the involvement of singlet oxygen in many damaging photoxidations in biological systems [9,10]. This is referred to as "photodynamic action" when the change requires the combination of light, oxygen and sensitizing dyes. Organisms affected include viruses, fungi, membranes, algae, as well as multicellular plants, animals, and humans, etc. [11-16]. There has been much speculation on the role of singlet oxygen in the photodegradation of polymers such as plastics, rubbers and oils [17-20], and in the chemistry of polluted urban atmospheres [21]. Mechanisms involving singlet oxygen have been proposed for photocarcinogensis [22], for the treatment of neonatal jaundice, which involves irradiation with light absorbed by bilirubin [23], and in cancer therapy where the use of

[1]Figures in brackets indicate literature references.

sensitizing dyes (hematoporphyrins) together with red light irradiation has been reported to lead to "excellent" regression of human tumors in certain patients [24].

It is perhaps necessary, following such an impressive list of important reactions possibly attributable to singlet oxygen, to stress once more that there are several established mechanisms for photo-oxidation [25–28]. Two major classes of photosensitized oxygenations have been designated as Type I and Type II [29–30]. In the former the sensitizer interacts directly with the substrate resulting, for example, in either H-atom or electron transfer. The radicals so produced from the sensitizers react in the presence of oxygen to regenerate the sensitizers while radicals produced from the substrate, for example initiate free radical chain reactions, as observed in auto-oxidations, etc. Type II reactions involve the direct interaction of the excited sensitizer with oxygen which upon energy transfer gives singlet oxygen or following electron transfer produces the superoxide ion, O_2^- [9,30].

The extent of interest in singlet oxygen may be judged by the numerious recent reviews and conferences dealing with singlet oxygen [e.g., 8,9,10,30–36]. It was thus considered timely to compile a comprehensive and critical review of rate constants for decay and reaction of singlet oxygen in fluid solution. The literature has been searched thoroughly up to the end of 1978 and many 1979 papers are included.

2. The Decay of Singlet Oxygen

The ground electronic state of molecular oxygen, which has zero angular momentum about the internuclear axis and contains two unpaired p electrons, has the group theoretical symbol $^3\Sigma_g^-$. The two electronically excited singlet states which arise from the same electron configuration but with spin pairing of these two electrons are the $^1\Delta_g$ and the $^1\Sigma_g^+$ states which lie 95 and 158 kJ mol^{-1} respectively above the $^3\Sigma_g^-$ ground state. The electronic transitions $^1\Delta_g \leftarrow {}^3\Sigma_g^-$ and $^1\Sigma_g^+ \leftarrow {}^3\Sigma_g^-$ although highly forbidden are readily observed in absorption and emission in the upper atmosphere and estimated radiative lifetimes of 64 min and 10 s, respectively, have been reported [37–38]. The measured lifetimes in the gas phase and in solution are very much shorter than this. In fact, in condensed media, the lifetime of $O_2^*(^1\Sigma_g^+)$ is so short that virtually nothing is known about its properties, and thus the term singlet oxygen is used throughout this review to refer to the $^1\Delta_g$ state.

In the gas phase $O_2^*(^1\Delta_g)$ can be studied by several methods, e.g., using its emission spectrum, or its ESR spectrum, by calorimetry, by photoionization or by chemical methods, but only the latter method was feasible in fluid solution until very recently when the photoinduced luminescence of $O_2^*(^1\Delta_g)$ was observed in air saturated solutions [39,40]. Singlet oxygen is produced rapidly following pulsed excitation and its kinetic behaviour can be deduced by allowing it to react with an acceptor A. Decrease in the absorption of A can be monitored over a time period of several half-lives. Analysis of the direct kinetics of disappearance of the acceptor gives information concerning the *first* order decay of singlet oxygen as well as the second order rate constant for its reaction with the acceptor. This method was evolved by Adams and Wilkinson [41] who used laser excitation of a sensitizer, S (e.g. methylene blue) to give its triplet state which in "aerated" fluid solution is rapidly quenched by molecular oxygen to produce singlet oxygen and the kinetics of its reaction with an absorbing acceptor, 1,3-diphenylisobenzofuran (DPBF), was followed spectrophotometrically at the absorption maximum of this acceptor. The various workers who have applied this method have used slightly different methods of kinetic analysis as outlined below [41–44].

2.1. Kinetic Analysis of the Disappearance of an Oxidizable Acceptor A Following Pulsed Excitation of a Sensitizer S

Consider the following mechanism which constitutes part of the general kinetic scheme given in Appendix I.

1 $\quad S + h\nu \longrightarrow {}^1S^* \longrightarrow {}^3S^*$; with rate $= I_a\Phi_T^{O_2}$

2 $\quad {}^3S^* + {}^3O_2(^3\Sigma_g^-) \longrightarrow {}^1O_2^*(^1\Delta_g) + S\ (k_{T\Delta})$

3 $\quad {}^1O_2^*(^1\Delta_g) \longrightarrow {}^3O_2(^3\Sigma_g^-)\ (k_d)$

4 $\quad {}^1O_2^*(^1\Delta_g) + A \longrightarrow AO_2$ or other products (k_r^A)

5 $\quad {}^1O_2^*(^1\Delta_g) + A \longrightarrow A + {}^3O_2(^3\Sigma_g^-)$; physical quenching$(k_q^A)$

where I_a is the rate of absorption of photons by S and $\phi_T^{O_2}$ is the quantum yield of triplet state production of the sensitizer in the presence of dissolved oxygen and rate constants are given in brackets following each step. In addition γ_Δ is the fraction of singlet oxygen produced for each sensitizer triplet quenched by oxygen with rate constant k_{T0}, i.e. $\gamma_\Delta = k_{T\Delta}/k_{T0}$ and $k_r^A + k_q^A = k_A$, the rate constant for quenching of singlet oxygen by A by both reaction and physical quenching. When excitation is by a pulse of $\sim$20 ns duration it follows, since $k_{T0}[O_2]$ in aerated solutions is usually in the range 3×10^6 to 3×10^7 s^{-1}, that after ~ 1 μs steps *1* and *2* above will be more than 95% complete so that, after this time, singlet oxygen decay will be given by

$$-d[^1O_2^*]/dt = (k_d + k_A[A])[^1O_2^*] \quad (1)$$

and therefore

$$[^1O_2^*] = [^1O_2^*]_{t=0}[\exp-(k_d t + \int_0^t k_A[A]dt)]. \quad (2)$$

From reaction *4*

$$-d[A]/dt = k_r^A[A][^1O_2^*] \quad (3)$$

and therefore

$$-d[A] = k_r^A[A][^1O_2^*]_{t=0}[\exp-(k_d t + \int_0^t k_A[A]dt)]dt \quad (4)$$

Equation (4) has been treated slightly differently as follows:

(a) Merkel and Kearns [42,43] assumed [A] on the right hand side of eq (4) can be treated as constant (i.e. as $[A]_{av}$ since typically [A] only varies by ~10%) and then integration of eq (4) gives, taking $k_D = k_d + k_A[A]_{av}$.

$$[A] - [A]_\infty = (k_r^A[^1O_2^*]_{t=0}[A]_{av}/k_D)[\exp(-k_D t)] \quad (5)$$

Since the change in concentration of A is proportional to ΔA, the change in absorbance by the oxidizable acceptor at some convenient wavelength, i.e.

$$[A]_t - [A]_\infty = \Delta A/\epsilon l, \quad (6)$$

where ϵ is the extinction coefficent and l the analyzing path-length, it follows from eqs (5) and (6) that a plot of $-\ln \Delta A$ vs t should have a slope equal to $k_D = k_d + k_A[A]_{av}$. Thus by varying $[A]_{av}$ values of k_d and k_A can be determined.

(b) Adams and Wilkinson [41] and Young, et al. [44] replaced [A] only in the exponential term in eq (4) by $[A]_{av}$ and then integrated eq (4) to give

$$\ln([A]/[A]_0) = (k_r^A[^1O_2^*]_{t=0}/k_D)[\exp(-k_D t) - 1] \quad (7)$$

or

$$\ln([A]/[A]_\infty) = (k_r^A[^1O_2^*]_{t=0}/k_D)[\exp(-k_D t)] \quad (8)$$

Experimental results were fitted to eqs (7) or (8) to evaluate k_D and thus values of k_d and k_A were obtained.

Comparison of the values obtained from the same data for k_D using eqs (5) or (7) and (8) give agreement to within ±5% and do not differ, within an experimental error of about ±10% when experiments are repeated many times, from time consuming computer treatments which do not make any assumptions about [A] being relatively constant.

In the presence of a singlet oxygen quencher Q, i.e. including the steps *6* and *7*,

6 $^1O_2^*(^1\Delta_g) + Q \rightarrow O_2(^3\Sigma_g^-) + Q\ (k_q^Q)$

and

7 $^1O_2^*(^1\Delta_g) + Q \rightarrow QO_2$ or other products (k_r^Q),

eq (1) becomes

$$-d[^1O_2^*]/dt = (k_d + k_A[A] + k_Q[Q])[^1O_2^*] \quad (9)$$

where $k_Q = k_r^Q + k_q^Q$ and k_D the decay constant for singlet oxygen now in the presence of a quencher becomes

$$k_D = k_d + k_A[A] + k_Q[Q]. \quad (10)$$

Measurement of k_D as a function of [Q] allows values of k_Q to be obtained. N.B. If k_Q is partly due to physical quenching and partly due to reaction, the value of k_Q obtained will be the total rate constant for quenching due to both processes.

A variation on this method has been developed by Matheson, et al. [45] in which singlet oxygen is directly generated by absorption of the output at 1065 nm of a pulsed Nd–glass laser by oxygen dissolved under pressure (up to 130 atm) in 1,1,2–trichlorotrifluoroethane (Freon 113). The disappearance of the singlet oxygen acceptor DPBF was monitored. Because of the high concentration of oxygen present, quenching by ground state oxygen, i.e. due to the reaction *8*,

8 $^1O_2^*(^1\Delta_g) + {}^3O_2(^3\Sigma_g^-) \rightarrow 2O_2(^3\Sigma_g^-)\ (k_q^{O2})$,

contributes substantially to singlet oxygen decay. Thus under these conditions eqs (5) to (8) apply and

$$k_D = k_d + k_A[A] + k_q^{O2}[O_2].$$

However since under these conditions $k_q^{O2}[O_2] >> k_d$ only values of $k_A[A]$ and k_q^{O2} can be obtained by measuring k_D as a function of [A] or $[O_2]$ respectively.

2.2. Kinetic Analysis of the Decay of Triplet β–Carotene Produced by Energy Transfer from Singlet Oxygen

Farmilo and Wilkinson [46] have developed a method for measuring singlet oxygen decay which monitors absorption by triplet β–carotene, $^3C^*$, formed in aerated solutions containing a sensitizer and a low concentration of β–carotene. Consider the mechanisms given above in the absence of A but in the presence of β–carotene, C, i.e. a mechanism which includes steps *1*, *2*, *3*, *6* and *7* together with steps *9* to *12* given below

9 $^3S^* + C \rightarrow {}^3C^* + {}^1S\ (k_{TC})$

10 $^1O_2^*(^1\Delta_g) + C \rightarrow {}^3C^* + {}^3O_2(^3\Sigma_g^-)\ (k_{\Delta C})$

11 $^3C^* \rightarrow C\ (k_{dC})$

12 $^3C^* + {}^3O_2(^3\Sigma_g^-) \rightarrow$ quenching (k_{CO})

The differential rate equations which can be written for $d[^3S^*]/dt$, $d[^1O_2^*]/dt$ and $d[^3C^*]/dt$ can be solved without making the steady–state approximation and this gives the concentration of $[^3C^*]$ as

$$[^3C^*] = U[\exp(-k_T t) - \exp(-k_C t)] + V[\exp(-k_D t) - \exp(-k_C t)] \quad (11)$$

where $k_T = k_{TO}[O_2] + k_{TC}[C]$; $k_C = k_{CO}[O_2] + k_{dC}$, and $k_D = k_d + k_{\Delta C}[C] + k_Q[Q]$. In aerated solutions the values of $k_{TO}[O_2]$ and $k_{CO}[O_2]$ are such that after ~1 μs, $\exp(-k_T t)$ and $\exp(-k_C t)$ become negligibly small and eq (11) becomes

$$[^3C^*] = V \exp(-k_D t) \quad (12)$$

where $V = [^3S^*]_{t=0} k_{\Delta C}[C] k_{T0}[O_2]/[(k_T - k_D)(k_C - k_D)]$. V is a constant provided $[O_2]$, [C] and [Q] are constant. It is usually possible to arrange for these to be present in excess so that $[O_2] >> [^1O_2^*]$, $[C] >> [^3C^*]$ and any consumption of Q or O_2 must also be negligibly small. It is important to bear these conditions in mind especially for work which involves for example focussed, high-energy, laser pulses. However when these conditions are met it follows from eq (12) that the decay of triplet β-carotene after $\sim 1\ \mu s$ becomes first order with a decay constant k_D equal to that of its precursor, singlet oxygen as confirmed by Farmilo and Wilkinson [46]. Thus the decay of absorption at 520 nm due to $^3C^*$ under these conditions mirrors the singlet oxygen decay yielding values of k_D and hence values of k_d, $k_{\Delta C}$ and k_Q. Only a few values of k_d and k_Q have so far been obtained using this method [46–48].

2.3. Photoluminescence of Singlet Oxygen in Solution

By using a mechanical phosphoroscope Krasnovsky has been able to detect luminescence from $O_2^*(^1\Delta_g)$ following energy transfer to oxygen from the triplet states of various sensitizers [40]. The weak emission at 1270 nm has a maximum lifetime τ in CCl_4 of 28 ms and a phosphorescence yield of 5×10^{-5}. This lifetime is considerably longer than those by other methods (see entry 1.8 and section 5). Also the radiative lifetime calculated from these measurements of 560 s in CCl_4 is about seven times less than the estimated radiative lifetime in the gas phase [37], however, this difference could result from solvent perturbation.

Krasnovsky has shown that in the presence of a singlet oxygen quencher Q the luminescence yield of singlet oxygen decreases and this decrease follows a Stern–Volmer relationship, i.e.

$$\phi_0/\phi = 1 + k_Q\tau_0[Q] = 1 + [Q]/\beta_Q \quad (13)$$

where ϕ_0 and ϕ are the phosphorescence yields of $O_2^*(^1\Delta_g)$ in the absence and presence of the quencher. From the slopes of the linear Stern–Volmer plot, taken together with the measured τ_0, i.e. the lifetime of $O_2^*(^1\Delta_g)$ phosphorescence in the absence of quencher, Krasnovsky gets values of k_Q in good agreement with other workers (see entries 2.130, 4.28, 5.26, and 6.40).

3. Kinetic Analysis for Sensitized Photo-oxygenations Using Irradiation with Continuous Light Sources

A full kinetic scheme which includes most possible elementary reactions for even the most perverse Type II sensitized photo-oxygenation involving singlet oxygen is shown in figure 1 and given in the table in Appendix I. In the vast majority of the systems cited in this review almost all of the steps involving interaction with the excited singlet and triplet states of the sensitizer with the exception of oxygen quenching have been shown to be absent. In fact one of the criteria for choosing a sensitizer is the absence of such complications. However, whenever experimental conditions are changed markedly by using different types of sensitizers or highly reactive quenchers, high concentrations, intensities etc., it is perhaps as well to bear in mind the number of complicating possibilities as illustrated in the table in Appendix I.

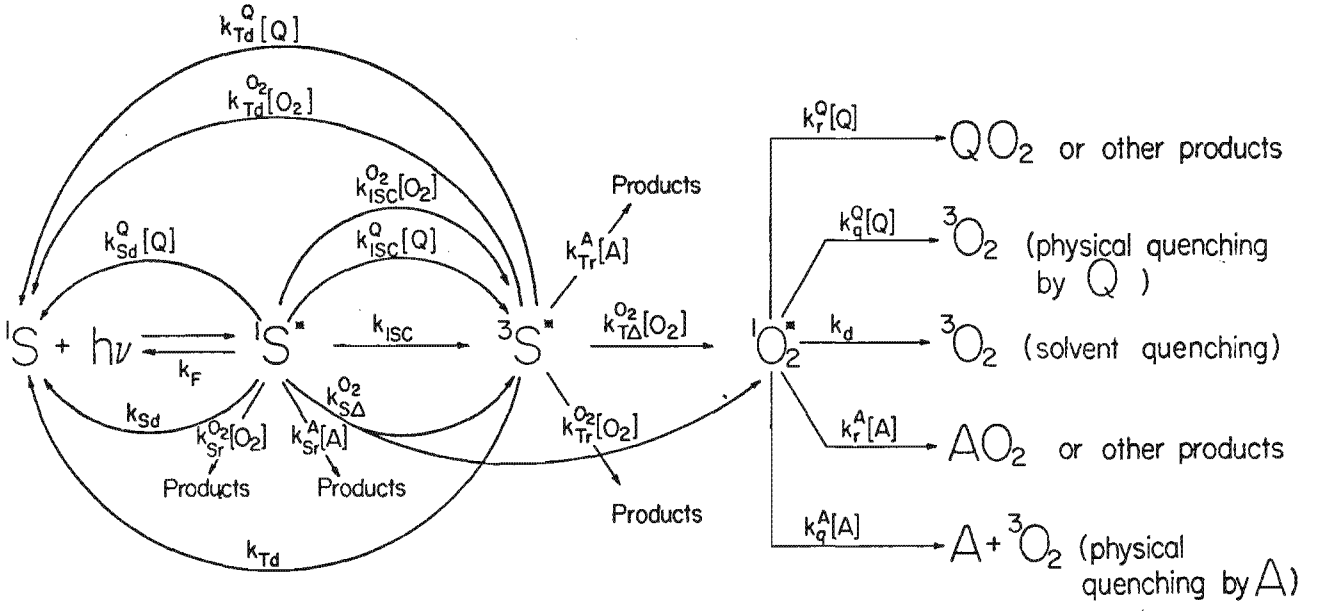


FIGURE 1. Kinetic scheme for the photosensitized formation of singlet molecular oxygen. S = sensitizer, A = oxidizable substrate, Q = physical quencher.

3.1. Sensitized Photo-oxygenation of a Single Substrate A

Many photosensitized reactions have been carried out under conditions such that no quenching by A of the sensitizer singlet or triplet states occurs, in which case the mechanism can be simplified to steps *1–5* as given in section 2.1. For continuous irradiation the steady-state approximation can be applied to steps *1–5* to give

$$\text{Rate of oxygenation} = r_{ox} = I_a\phi_T^{O_2}\gamma_\Delta k_r^A[A]/(k_d + k_A[A]) \quad (14)$$

where the rate of oxygenation may be followed by determining the rate of production of some product and/or the rate of disappearanc of either the substrate A and/or of oxygen. All three have been used and this is indicated in the tables by an entry in the methods column. N.B. It follows from eq (14) that when $k_d >> k_A[A]$ or $k_A[A] >> k_d$ the rate of oxygenation will be first or zero order with respect to A respectively. Equation (14) can be rearranged to give

$$r_{ox}^{-1} = (I_a\phi_T^{O_2}\gamma_\Delta\gamma_r^A)^{-1}\,[1 + (k_d/k_A)(1/[A])] \quad (15)$$

where $\gamma_r^A = k_r^A/k_A$ is the fraction of reactive quenching of singlet oxygen by A. According to eq (15) linear plots of r_{ox}^{-1} vs $[A]^{-1}$ should give

$$\text{slope/intercept} = k_d/k_A = \beta_A,$$

where $\beta_A = k_d/k_A$ represents the concentration at which the decay of singlet oxygen in the solvent alone (step *3* equals the decay due to quenching by A (steps *4* and *5*) i.e. it is the half-quenching concentration. (N.B. Equation (15) only predicts a linear relationship if there is (i) constant light intensity, (ii) constant absorption by the sensitizer (no absorption by A although this could be allowed for), and (iii) a constant oxygen concentration in the solution.)

Tables 2 to 15 list hundreds of β values many of which were determined before absolute values of k_d were reported, in which case we have taken preferred values of k_d from table 1 in order to derive values of k_A from these β values. Where authors have quoted values of k_A derived in like manner we have quoted the values of k_d they used in the comments column of the tables. When the use of preferred values for k_d gives a value of k_A differing by more than the quoted experimental error or by more than 25% this value is also given in brackets and marked with an asterisk.

3.2. Photo-Auto-Oxygenation of a Single Substrate A

When a substrate acts as its own sensitizer yielding singlet oxygen one can observe Type II photo-auto-oxygenations. Good examples are rubrene(Rub) and 9,10-dimethylanthracene(DMA) and for such cases this is indicated in the comments column of the tables by S = self. Since the self-sensitizer is consumed in the photo-auto-oxygenation this usually leads to a change in I_a which must be allowed for. Alternatively, a totally absorbing solution can be used and then the rate of production of some product or the rate of consumption of oxygen can be measured and substituted directly into equation (15) to obtain values of β since under these conditions I_a is effectively constant.

3.3. Sensitized Photo-Oxygenations of a Substrate A in the Presence of a Second Substrate A′ which also Reacts with Singlet Oxygen

Consider in addition to steps *1* to *5* the further steps *13* and *14*

13 $\quad {}^1O_2{}^*({}^1\Delta_g) + A' \rightarrow A'O_2$ or other products $(k_r^{A'})$

14 $\quad {}^1O_2{}^*({}^1\Delta_g) + A' \rightarrow A + {}^3O_2\ (k_q^{A'})$

(We prefer to use A′ rather than Q (see steps *7* and *8*) for an additive which is known to react chemically with singlet oxygen).

In the presence of a second substrate [A′] it follows that

$$-d[A']/dt = I_a\phi_T^{O_2}\gamma_\Delta k_r^{A'}[A']/(k_d + k_A[A] + k_{A'}[A']),$$

which when $k_{A'}[A'] << (k_d + k_A[A])$ becomes

$$-d\ \ln[A']/dt = I_a\phi_T^{O_2}\gamma_\Delta k_r^{A'}/(k_d + k_A[A]) = S,$$

where S is the slope of the first order plot from the disappearance of A′. In the absence of A under identical conditions

$$-d\ \ln[A']/dt = I_a\phi_T^{O_2}\gamma_\Delta k_r^{A'}/k_d = S_0.$$

thus

$$S_0/S = 1 + (k_A/k_d)[A] = 1 + [A]/\beta_A. \quad (16)$$

Young and coworkers [48,49] and others [50,51] have used this Stern-Volmer equation to obtain β values using the highly reactive fluorescent substrate 1,3-diphenylisobenzofuran (DPBF) as A′. This substrate is more reactive than most (see tables 2 to 15) so that it decays in a first order manner during continuous irradiation in photosensitized oxidation experiments even in the presence of other substrates. The low concentrations of DPBF are often monitored by following the decrease in its fluorescence. Note that when $k_q^A >> k_r^A$ (i.e. if A were a physical quencher of singlet oxygen) equation (16) applies even for much less reactive substrates than DBPF.

Application of the steady-state approximation to steps *1* to *5* together with *13* and *14* gives

$$(d[AO_2]/dt)/(d[A'O_2]/dt) = (-d[A]/dt)/(-d[A']/dt) = k_r^A[A]/k_r^{A'}[A'] \quad (17)$$

which upon integration gives

$$\ln([A]_0/[A])/\ln([A']_0/[A']) = k_r^A/k_r^{A'}.$$

Equation (17) and its integrated forms have been used to determine values of $\beta_r = k_d/k_r^A$. Equation (17) can also be used to compare rates of oxidation of two substrates A and A′ separately irradiated under identical conditions in the same solvent for example as in 'merry-go-round' experiments, and to compare the rates of the same substrate in different solvents (for examples see [49]).

Alternatively, $r_{ox}^{A'}(A)$ and $r_{ox}^{0}(A)$, the rates of oxygenation of A in the presence and absence of A′ respectively, can be evaluated and these will be related by the equation,

$$(r_{ox}^{0}(A)/r_{ox}^{A'}(A))_{t=0} = 1 + ([A']_0/\beta_{A'})(1 + [A]_0/\beta_A)^{-1} \quad (18)$$

provided A′ does not absorb any exciting light, quench or react with $^1S^*$ or $^3S^*$. If initial rates are measured keeping [A′] constant and varying $[A']_0$ then eq (18) allows values of $\beta_{A'}$ to be obtained. Alternatively if $\beta_A >> [A]_0$ eq (18) simplifies allowing the determination of $\beta_{A'}$ values.

3.4. Sensitized Photo-Oxygenations of a Substrate A in the Presence of Q, a Physical Quencher of Singlet Oxygen

Consider steps *1* to *6*, i.e. assuming for the moment there is no reaction with singlet oxygen by the quencher Q and that it does not absorb the exciting light. Application of the steady-state approximation then predicts

$$(r_{ox}^{Q})^{-1} = (I_a\phi_T^{O2}\gamma_\Delta\gamma_r^A)^{-1}[1 + [A]^{-1}(\beta_A + k_Q[Q]/k_A)] \quad (19)$$

i.e. a linear relationship between $(r_{ox}^{Q})^{-1}$ and $[A]^{-1}$ with

$$\text{slope/intercept} = (\beta_A + k_Q[Q]/k_A) \quad (20)$$

In the absence of quencher slope/intercept $= \beta_A$ (see also eq (15). Thus

$$(\text{slope/intercept})_Q/(\text{slope/intercept})_0 = 1 + k_Q[Q]/k_d = 1 + \beta_Q^{-1}[Q]. \quad (21)$$

In the absence of quenching of excited singlet and triplet states of the sensitizer the intercepts of $(r_{ox}^{Q})^{-1}$ vs $[A]^{-1}$ plots are identical and it follows from equation (19) and/or (21) that that

$$(\text{slope})_Q/(\text{slope})_0 = 1 + \beta_Q^{-1}[Q] \quad (22)$$

In addition from eq (19) the ratio of the rates of oxygenation in the absence and presence of Q is given by

$$(r_{ox}^{0}/r_{ox}^{Q})_{t=0} = 1 + k_Q[Q]/(k_d + k_A[A]_0) = 1 + ([Q]/\beta_Q)(1 + [A]_0/\beta_A)^{-1} \quad (23)$$

cf. eq (18). Alternatively if one assumes [A] does not change appreciably (i.e. for low fraction conversions) eq (19) can be integrated to give after time t

$$[AO_2]_0/[AO_2] = [A]_0/\Delta[A] = A^0/\Delta A = (I_a t\phi_T^{O2}\gamma_\Delta\gamma_r^A)^{-1}([A]_0 + k_d/k_A + k_Q[Q]/k_A) \quad (24)$$

where ΔA represents the change in the absorbance by the reactant A. Plots of $A^0/\Delta A$ vs [Q] have been shown to be linear and from eq (24) it follows that for such plots

$$k_Q = (\text{slope/intercept})(k_d + k_A[A]_0) \quad (25)$$

3.5. Sensitized Photo-Oxygenation of a Substrate A in the Presence of a Quencher of Both Singlet Oxygen and the Sensitizer Triplet

The mechanism is now that given by steps *1* to *6* together with the reaction *15*

15 $\quad ^3S^* + Q \rightarrow S + Q \text{ or } Q^* \ (k_{QT})$

Application of the steady-state approximation gives

$$(r_{ox}^{Q})^{-1} = (I_a\phi_T^{O2}\gamma_\Delta\gamma_r^A)^{-1} \times (k_{QT}[Q]/k_{TO}[O_2] + 1)[1 + [A]^{-1}(\beta_A + k_Q[Q]/k_A)] \quad (26)$$

Note that for a plot of $(r_{ox}^{Q})^{-1}$ vs $[A]^{-1}$ the slope/intercept is still given by eq (20) as the extra term in eq (26) affects both the intercept and slope equally. The presence or absence of this change in intercept for $(r_{ox}^{Q})^{-1}$ vs $[A]^{-1}$ plots can be used as a diagnostic test for the presence of steps such as *15* which reduce the yield of singlet oxygen produced for potential reaction. Another test is the occurence of a dependence on the concentration of oxygen in solution since reaction *15* competes with reaction *2* and thus the yield of singlet oxygen becomes dependent on the pressure of oxygen above the solution. (e.g. see [52,53]).

3.6. Separation of k_r and k_q

Apart from equation (17) application of all of the equations given so far only allows values of $k_A = k_r^A + k_q^A$ or $k_Q = k_r^Q + k_q^Q$ to be obtained. Methods which have been used to separate k_r and k_q values usually involve the direct measurement of the quantum yields of oxygenation, ϕ_{AO2}, for example at high concentrations of A such that $k_A[A] >> k_d$, in which case it follows from equation (14) that

$$(\phi_{AO2})_{[A]\rightarrow\infty} = \phi_T^{O2}\gamma_\Delta\gamma_r^A. \quad (27)$$

Often the limiting yield of oxygenation of a very reactive acceptor e.g. α–terpinene or dimethylfuran for which γ_r^A is close to unity (i.e. $k_r^A >> k_q^A$) is used as a reference substrate to give values of $\phi_T^{O_2}\gamma_\Delta$ and whence γ_r^A for other additives (e.g. see [54,55]). Alternatively at low values of [A] when $k_d >> k_A[A]$ eq (14) gives

$$\phi_{AO_2} = \phi_T^{O_2}\gamma_\Delta k_r^A[A]/k_d \quad (28)$$

and measurement of ϕ_{AO_2} together with a knowledge of $\phi_T^{O_2}$, γ_Δ and k_d or β_A allows values of k_r^A or γ_r^A to be determined.

4. Kinetic Analysis for Oxygenation by Singlet Oxygen Generated by Chemical Reaction, by Microwave Discharge, or by Direct Laser Excitation

4.1. Chemical Production of Singlet Oxygen

Oxygenation reactions arising from singlet oxygen produced chemically have been studied in the presence and absence of singlet oxygen quenchers. Among the reactions used to form singlet oxygen are (a) reaction of hydrogen peroxide with hypochlorite or hypobromite, (b) reaction of potassium superoxide with water, and (c) thermal decomposition of aryl peroxides or of the ozonide of triphenyl phosphite. Experiments are usually carried out so that a fixed amount of singlet oxygen is produced in the presence of variable amounts of reactive substrate A and/or A′ with or without added quencher, Q.

In the absence of quencher the decrease in A is given by the relative probabilities of steps *3*, *4*, and *5* (section 2) i.e.

$$-d[A]/dt = (d[^1O_2{}^*]/dt)[k_r^A[A]/(k_d + k_A[A])] \quad (29)$$

which integrates to give

$$\beta_A \ln([A]_0/[A]_\infty) + [A]_0 - [A]_\infty = \gamma_r^A[^1O_2{}^*]_\infty \quad (30)$$

where $[^1O_2{}^*]_\infty$ is the total amount of singlet oxygen generated chemically. For small fractional conversions $\ln([A]_0/[A]_\infty) = ([A]_0 - [A]_\infty)/[A]_\infty$ and substitution into (30) gives upon rearrangement

$$1/\Delta[A] = (\gamma_r^A[^1O_2{}^*]_\infty)^{-1}[(\beta_A/[A]_\infty) + 1] \quad (31)$$

where $\Delta[A] = [A]_0 - [A]_\infty$. Thus a plot of $\Delta[A]^{-1}$ vs $[A]^{-1}$ for small conversions has slope / intercept $= \beta_A$. In the presence of a quencher eq (30) becomes

$$(\beta_A + k_Q[Q]/k_A)(\ln[A]_0/[A]_\infty + \Delta[A]) = \gamma_r^A[^1O_2{}^*]_\infty \quad (32)$$

so that if k_d and k_A are known eq (32) allows k_Q to be evaluated from values of $[A]_0$ and $[A]_\infty$ in the presence of [Q]. With the decomposition of the ozonide $(C_6H_5O)_3P...O_3$ in the presence of pyridine, Mendenhall [56] has shown that there is quantitative generation of $^1O_2{}^*$ so that $[^1O_2{}^*]_\infty$ can be replaced by the initial concentration of $(C_6H_5O)_3PO_3$, i.e. $[^1O_2{}^*]_\infty = [(C_6H_5O)_3PO_3]_0$ and γ_r^A is often assumed to be unity when A is rubrene[57].

4.2. Microwave Generation of Singlet Oxygen

When a microwave discharge is passed through oxygen gas in a gaseous flow system singlet oxygen ($^1\Delta_g$ and $^1\Sigma_g^+$), oxygen atoms, and ozone are produced. The latter two oxidizing species can be removed by reaction with mercury vapour and the $O_2{}^*(^1\Sigma_g^+)$ will be rapidly quenched, probably to give $^1O_2{}^*(^1\Delta_g)$ when the emerging gases are bubbled through solutions containing oxidizable substrates. Often the flow is bubbled simultaneously through two cells, one containing the substrate only and the other substrate and potential singlet oxygen quencher. This makes it easier to allow for variation in the concentration of dissolved oxygen produced in these bubbling experiments. Equations (29) to (32) also apply to the disappearance of a substrate as a result of reaction of singlet oxygen generated in microwave experiments or for that matter for singlet oxygen produced via photosensitization. Taking eq (32) for relative measurements with the same initial concentration of substrate $[A_0]$ in the presence and absence of a quencher gives

$$k_Q = [k_A([A]_\infty^Q - [A]_\infty^0) + k_d\ln([A]_\infty^Q/[A]_\infty^0)]/[Q]\ln([A]_0/[A]_\infty^Q) \quad (33)$$

where $[A]_\infty^Q$ and $[A]_\infty^0$ represent the final values after exposure to microwave generated singlet oxygen in the presence and absence of quencher respectively.

4.3. Direct CW Laser Production of Singlet Oxygen

Evans and Tucker [58, 59] and Matheson and Lee [45, 60, 61] have used laser excitation of highly concentrated oxygen solutions in high pressure cells, with gaseous oxygen up to 130 atm, to give directly the $^1O_2{}^*(^1\Delta_g)$ state by absorption at 1065 nm from a CW Nd YAG laser and $^1O_2{}^*(^1\Delta_g)$ directly from the 'double transition' using He–Ne laser excitation at 632.8 nm. Evans and Tucker [59] find the quantum yields of photo–oxygenation of 9,10–dimethylanthracene and tetraphenylcyclopentadiene are twice as high for absorption of a photon in the 'double transition' as for the direct excitation of a single $^1\Delta_g$ state. Modification of eq (15) to account for the direct excitation by replacing $\phi_T^{O_2}\gamma_\Delta$ by $n = 1$ or 2 for excitation at 1065 nm or 633 nm respectively gives

$$1/\phi_{AO_2} = [(k_A/k_r^A) + (k_d/k_r^A[A])]/n \quad (34)$$

and plots of $\phi_{AO_2}^{-1}$ vs $[A]^{-1}$ can be used to give γ_r^A and β_A values [59].

Matheson, et al. [45,60,61] have obtained experimental pseudo first order rate constants for the disappearance of

various substrates while directly producing $O_2^*(^1\Delta_g)$ with a CW Nd YAG laser. Since the absorption involves the process

$$16 \quad 2\,^3O_2(^3\Sigma_g^-) + h\nu \rightarrow {}^1O_2^*(^1\Delta_g) + {}^3O_2(^3\Sigma_g^-)$$

eq (14) has been modified by them to give

$$-d[A]/dt = \sigma E[O_2]^2 k_r^A[A]/(k_d + k_A[A] + k_{O_2}[O_2]) \quad (35)$$

where E is the laser intensity and σ the absorption cross section for process *16*. At high oxygen concentration where $k_{O_2}[O_2] >> (k_d + k_A[A])$ the observed first order rate constant k_1 is given by

$$k_1 = \sigma E[O_2] k_r^A / k_{O_2}. \quad (36)$$

Thus from a knowledge of σ, E and $[O_2]$ values of k_r^A relative to k_{O_2} can be obtained. In the presence of singlet oxygen quencher at relatively high concentration

$$k_1 = \sigma E[O_2]^2 k_r^A / (k_{O_2}[O_2] + k_Q[Q]) \quad (37)$$

and a plot of $([O_2]/k_1)$ vs $([Q]/[O_2])$ will have a slope/intercept $= k_Q/k_{O_2}$.

Values obtained using this method have often been substantially lower than those given by other workers. According to Matheson and Toledo [62] this was due, partially at least, to an artifact with the over depletion of the acceptor concentration in the laser beam cross section so that the observed chemical reaction rate may be affected by diffusion of unreactive acceptor into the depleted region. Thus previous values in Freon 113 for k_r^A may be low by up to an order of magnitude.

5. First Order Rate Constants for the Decay of Singlet Oxygen in Various Solvents and Comments on Tables 1 and 1(a)

All the values given in table 1 were evaluated using the kinetic treatments outlined in sections 2.1, 2.2, and 2.3 (mostly 2.1). The solvents are arranged in order of increasing number of C atoms. If the number of carbon atoms is the same then the compounds are arranged in order of decreasing number of H atoms. When the number of C and H atoms are the same the arrangement is determined by the alphabetic order of the element symbols other than H.

Values of k_d in various solvents, usually at an unspecified temperature, which from the few studies of temperature dependence of k_d (see entries 1.5, 1.32, and 1.48) does not seem to affect the values to any great extent, are given in table 1 including errors as given in the original references. Unfortunately no indicator is usually given in the primary references as to the meaning of the error values which follow the $\pm$ signs, although occasionally standard deviations or 95% confidence limits are specified. The given error limits usually represent about 10–20% of k_d and in these circumstances we have assumed that most reported values are of similar accuracy. However if any research group gave a new value for k_d determined under virtually identical conditions we have ignored their earlier literature value in arriving at 'preferred' values. Only in the cases of benzene and methanol have a sufficient number of independent values been reported to allow us to average the reported values and statistically estimate 95% confidence limits of these average values. In all other cases except CCl_4 (see later) no more than three values have been reported and, unless any of these has been excluded as mentioned above or for other reasons given in the comments column, these have been averaged to give 'preferred' values. The reported values used to obtain the average values are indicated with double daggers. The average as 'preferred' values (indicated by asterisks in table 1) are used in figure 2 and for calculating further rate constants in subsequent tables (see later).

With benzene and methanol as solvent several values of k_d from a number of different research groups are available and agree to within $\pm$ 10%. However the discrepancies between the values of k_d in the cases of ethanol and chloroform, obtained by some of these same research groups amounts to factors of two to three! It is apparent therefore that the so called errors quoted within the references reflect the reproducibility of the values obtained and that large systematic errors sometimes occur. This suggests that where only one group has determined a value in a particular solvent it may only be within a factor of two of the true value although within a factor of one-half seems more likely. The same can be said for the averages of preferred values except for those given with 95% confidence limits. Such large systematic errors could be due to impurities in the solvents, e.g. 1% water in a solvent in which the decay rate is 100 times less than in water would double the value of k_d and even smaller amounts of more potent singlet oxygen quenchers (for likely candidates see tables 2 to 15) would produce similar effects. The lower the value of k_d the more critical is solvent purity. However the direct technique for measuring k_d depends on measuring k_D as a function of $[A]_{av}$ and when k_d is small although the slope of such a plot defines k_A quite precisely, large uncertainties in the intercepts, k_d, are likely. In such cases values of k_A measured directly in pulsed experiments can be combined with steady-state measurements of k_d/k_A (see section 3) to give more accurate values of k_d.

If the presence of impurities in solvents with low k_d is responsible for some of the differences observed it would also follow that the lower value is more likely to be the better value. However it is possible that, at the wavelengths used to monitor the disappearance of a substrate, weak overlapping transient absorption due for example to radicals from a small amount of type I photo-oxygenation could be superimposed. This could lead to inaccuracies in k_d in either direction depending on the nature of the transient. The presence of such artifacts could depend on intensity, wavelength, sensitizer, solvent, etc., and for this reason we have not automatically assumed the lowest reported value in a particular solvent to be the best.

In this connection the results of Krasnovsky [40] require

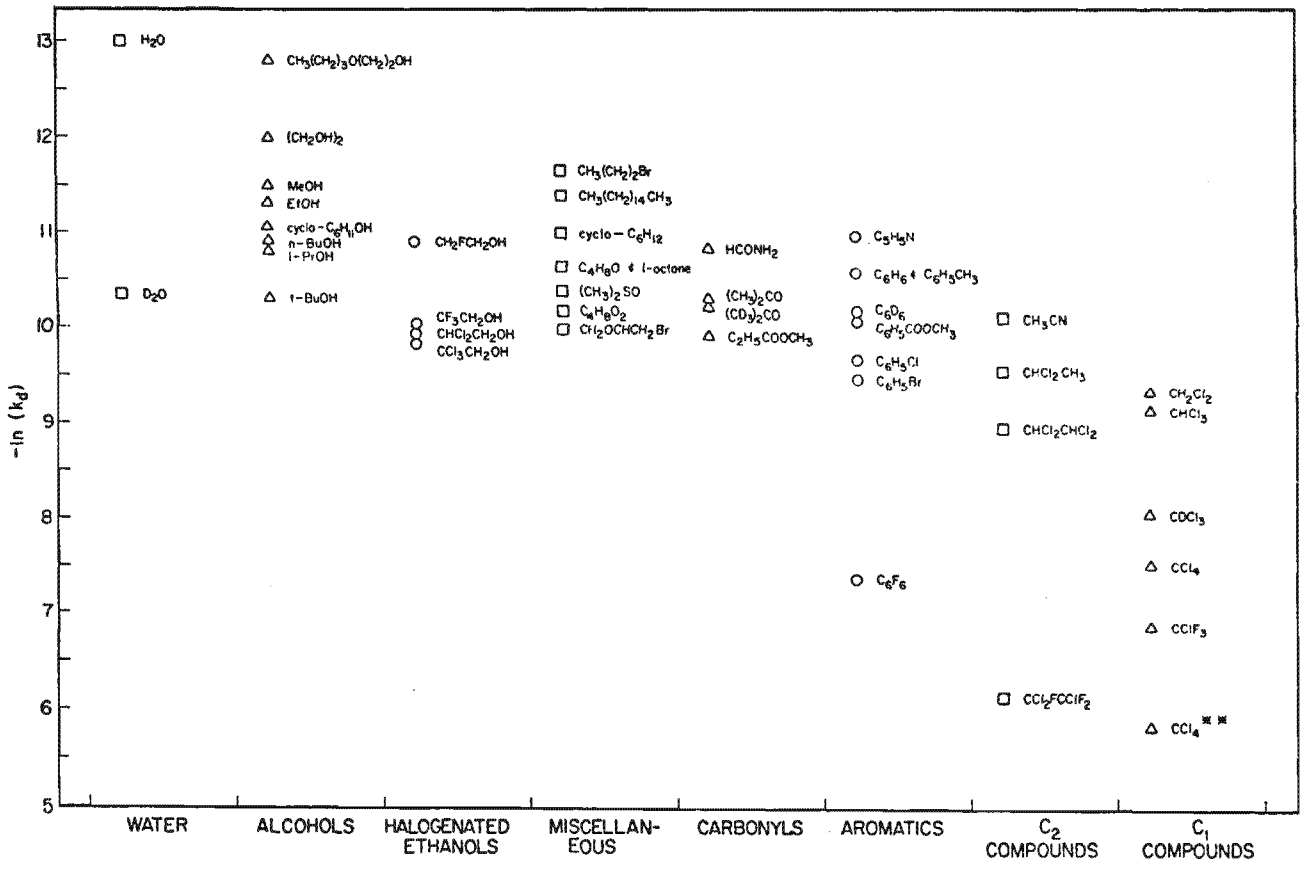


FIGURE 2. Plot of $-\ln(k_d)$ versus solvent class where k_d is the psuedo first order rate constant for physical deactivation of singlet oxygen by solvent molecules. ** Krasnovsky's value.

special comments. The method he uses is very direct since he measures emission from $O_2^*(^1\Delta_g)$. However the yield of the emission is very low and the transition lies in the infrared where experimental difficulties are considerable. Thus it is possible that his much longer lifetime ($\sim$50 times) for singlet oxygen in CCl_4 is due to some artifact. On the other hand the quenching constants he obtains based on this lifetime agree fairly well with those obtained by others in other solvents. In order to obtain this long lifetime Krasnovsky had to work at very low concentrations of sensitizers $\leqslant \mu M$ and this may give the clue to the differences observed. It could be that sensitizer quenching of singlet oxygen determines the measured lifetime in solvents where $k_d \leq 10^2$ s^{-1}. Krasnovsky [40] has measured singlet oxygen quenching rate constants of 10^6 and 4×10^7 dm^3 mol^{-1} s^{-1} respectively for tetraphenylporphine (TPP) and Zn^{2+}TPP both of which have been used as singlet oxygen sensitizers. Furthermore on the basis of the rate data given in this compilation it seems likely that many of the 'popular' sensitizers will have quenching constants as large as 10^5 dm^3 mol^{-1} s^{-1} (Even benzene, methanol and H_2O have quenching constants of about 3, 2 and 9×10^3 dm^3 mol^{-1} s^{-1}, respectively).

In the case of solvents where $k_d \leq 10^2$ s^{-1}, substantial quenching of singlet oxygen would be expected for sensitizer concentrations $> 10^{-4}$ mol dm^{-3}, and this could account for the different values of k_d reported by different research groups. Thus independent evaluation of Krasnovsky's results is needed as is a careful examination of the effect of change of concentration of sensitizer on the measured constant for singlet oxygen decay in solvents where $k_d \geq 10^2$ s^{-1}. In table 1 we have marked Krasnovsky's value of k_d in CCl_4 with two asterisks. It may be a 'best' value for k_d in CCl_4 however since the major application of k_d is to determine values of k_A or k_Q and since most photo-oxygenation studies have used sensitizers it follows that the value required for deriving k_A or k_Q is the decay constant in the absence of the substrates under comparable conditions. For this reason and the others outlined above we have not chosen Krasnovsky's value as a preferred value for combination with other data already in the literature.

Because of solubility problems mixed solvents are often used in photo-oxygenation experiments and values of k_d measured by the direct methods in some mixed solvents are included at the end of table 1. Furthermore, to overcome solubility problems with either the oxidizable acceptor (usually DPBF) or the sensitizing dye in some solvents, a small proportion of a co-solvent (often methanol) has been added and the decay constant k_D determined. Quenching by the co-solvent is then allowed for effectively by taking

$$k_D = k_d(\text{sol})X_{\text{sol}} + k_d(\text{co-sol})X_{\text{co-solvent}} + k_A[A]_{av} \quad (38)$$

where X_{sol} represents the mole fraction of the solvent, etc. This assumes that the contributions for decay of singlet oxygen by the co-solvent can be determined from k_d(co-sol), the decay constant in the neat co-solvent. Young and Brewer [64] have measured $k_{co\text{-}solvent}$, i.e. the singlet oxygen quenching rate constant for co-solvents, in carbon tetrachloride and found values only slightly lower than those calculated from eq (39),

$$k_{co\text{-}solvent} = k_d(\text{co-solvent})/[\text{neat co-solvent}] \quad (39)$$

(e.g. see values in tables 1 and 15). This confirms that only small errors are likely to be introduced by making use of equation (38) to extrapolate from k_D values determined in the presence of a small proportion of co-solvent to obtain a value of k_d in the solvent. If such an extrapolation has been used for data given in table 1, this is noted in the comments column by stating that values were corrected for the effect of x% of co-solvent.

For some solvents only estimates of the singlet oxygen decay constants have been published, i.e., so far they have not been measured directly by pulsed methods. Estimates are listed in table 1(a) for solvents not included in table 1. These estimated values for singlet oxygen decay constants are also included in figure 2. The assumptions made in arriving at these estimates e.g. that k_A(rubrene) $= 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} or that k_Q(β-carotene) is diffusion controlled are given in the comments column of table 1(a). Similar estimates have been made for solvents where the singlet oxygen decay constants have been measured by pulsed methods, e.g., by measuring β_A(rubrene) with chemical generation from $(PhO)_3PO_3$ decomposition and from the self-photosensitization of rubrene in dichloromethane, Carlsson et al. [63] obtained estimates of 7.3×10^3 s^{-1} and 9.5×10^3 s^{-1}, respectively, for the singlet oxygen decay constant in dichloromethane by assuming k_A(rubrene) $= 7.3 \times 10^7$ dm^3 mol s^{-1}. These values fall between the decay constants measured following pulsed excitation given in table 1 which are 7.1×10^3 s^{-1} and 1.6×10^4 s^{-1}. On the basis of the compilation made in this review it is possible to estimate somewhat different values for k_d and this has been done if considerably different estimates are indicated. Estimates have also been made for any solvents which have been used to measure singlet oxygen rate constants in which no published estimate is so far available.

The rate constants for the decay of singlet oxygen in fluid solutions can be seen to vary several hundredfold. Several reviewers have previously commented that the decay constants do not correlate with any of the following solvent parameters: viscosity, dielectric constant, ionization potential, polarity, polarizability, etc. However Merkel and Kearns [43], who have interpreted the solvent dependence of $^1O_2$* decay in terms of electronic to solvent vibrational energy transfer, have shown that

$$k_d/10^6 \text{ s}^{-1} \approx 0.5\, A_{7880} + 0.05\, A_{6280} \quad (40)$$

where A_{7880} and A_{6280} represent the absorbances of 1 cm of the solvent at 7880 cm^{-1} and 6280 cm^{-1} corresponding to the 0→0 and 0→1 vibrational components for $O_2(^3\Sigma_g^-) \leftarrow O_2^*(^1\Delta_g)$ transition. Young and Brewer [64] point out that this correlation is only moderately successful and suggest a better empirical relationship is obtained for a group of solvents (e.g., alcohols) by the equation

$$\ln k_d = a + b[\text{Ionization Potential}/(0.5\, A_{7880} + 0.05\, A_{6280})] \quad (41)$$

From the data given in table 1 and displayed in compound related groups in figure 2, it is apparent that the availability in the solvent molecule of high energy vibrations which can accommodate the considerable amount of energy which has to be converted from electronic to vibrational energy increases the decay constant observed. The replacement of hydrogen by deuterium usually gives decreased decay constants (e.g. D_2O/H_2O, C_6H_6/C_6D_6, $CDCl_3$ and $CHCl_3$) but no difference was observed by Merkel and Kearns [43] for the decay constant in acetone and acetone-d_6. Elimination of any X-H vibrations, where X is any element, from the solvent molecules usually results in a lowering of k_d.

6. Second Order Rate Constants for the Quenching of Singlet Oxygen by Various Substrates and Comments on Tables 2–15

Results concerning related groups of compounds e.g. olefins, aromatic hydrocarbons, aliphatic and cyclic amines etc. are separately collected in tables 2–15 in order of increasing structural complexity. A complete molecular formula index and in addition an alphabetically arranged chemical name index listing table entry numbers are also given to help with the location of various substrates in these tables. Apart from minor changes in table 10 all the headings to tables 2–15 are the same. The entry number is given in the first column, thus the first olefin in table 2 has an entry number 2.1 and further results on this substance in the same or different solvents are labelled 2.1.1, 2.1.2, 2.1.3, etc. Thus each result has a separate entry number and entry number 10.81.7 represents the eighth result on the 81st substrate in table 10. The second column names the substrate with its structural formula using drawings where necessary for clarity. The solvent is indicated in column 3 and the temperature where quoted is given in the sixth column (rt = room temperature). Where more than one solvent was used the results are listed with solvents in the same order as in table 1.

The rate constants for quenching of singlet oxygen by the substrate arising from both physical and chemical quenching are given in the fourth column except where separate reactive quenching rate constants (labelled k_r) or physical quenching rate constants (labelled k_q) were measured, i.e. $k = k_r + k_q$ except where otherwise stated in column 4.

Often the values of k, k_r or k_q are measured relative to other rate constants and this is indicated usually by giving

the primary measured ratio in the comments column except when this is a β value in which case the experimental value is given in column 5. In such cases the value of k, k_r or k_q depends on the relative literature value taken and this value is also given in the comments column with the table entry number for this value in this compilation given in square brackets. When preferred values taken from this compilation give values for k, k_r or k_q which differ by more than the quoted errors, or if none are quoted by more than 25%, the alternative value is also given and marked with an asterisk. The relative preferred value taken from this compilation in order to calculate this alternative value is given in brackets and marked with an asterisk. Thus for entry 2.1.1 the measured value is $\beta = (k_d/k) = (8.8 \pm 0.2) \times 10^{-1}$ mol dm^{-3} given in column 5 and $k = 4.3 \times 10^4$ dm^3 mol^{-1} s^{-1} using $k_d = 3.8 \times 10^4$ s^{-1} and *3.5×10^4 dm^3 mol^{-1} s^{-1} if the preferred value k_d (Av) = *3.1×10^4 s^{-1} is used. Both of these k_d values are to be found under entry 1.22, the first is the value given in [65] while the second is the average of this value and that obtained in [64] as given under entry 1.22.

The method used to obtain each result is indicated in column 7 by use of various two-letter abbreviations (see list of abbreviations) followed by a number which is the equation number in the text, use of which allows the determination of the cited experimental parameter. Thus entry number 3.1 has A'd-8 in the methods column. A'd stands for reference acceptor A' disappearance (see list of abbreviations) and implies that the authors monitored A' = DPBF (see comments column) disappearance as a function of time after exciting methylene blue as sensitiser (S = MB in comments column) in the presence of the substrate, benzene and by use of equation 8 obtained the value of k with errors as shown. As a further example consider entry 5.1 where the methods column entry is Od-15, thus by measuring the rate of oxygen disappearance (Od) with rose bengal as sensitizer (see comments column) and by the use of equation 15 a value of β given in the fifth column was obtained equal to 4.5×10^{-3} mol dm^{-3}. The value of k given in column 4 was derived using the k_d value taken from results given in entry 1.3.6 indicated by [1.3.6] in the comments column.

The final column in all 15 tables gives a reference as the first four letters in the first author's name followed by a period for each co-author together with the Radiation Chemistry Data Center serial number, the first two digits of which specify the year of publication. Thus, the data for entry 1.24 comes from a paper by Young, Brewer and Keller [44] published in 1973 and the reference column entry is Youn.. 73F014. A full list of references is given at the end of the tables in order of the Data Center serial number.

The scatter in the results is considerable, e.g. see entry 2.33 which gives seven values for k from three different laboratories for 2-methyl-2-butene in methanol. The values range from 1.7×10^5 to 3.3×10^6 dm^3 mol^{-1} s^{-1} and the two extreme values are from the same source [66]. The most studied substrate is 9,10-diphenylisobenzofuran and if one considers the nine results, entries 5.36.84 to 5.36.92 (from five different laboratories) where benzene was used as a solvent, the values of k range from $(3.5 \pm 1.3) \times 10^8$ to $(1.5 \pm 0.5) \times 10^9$ dm^3 mol^{-1} s^{-1}. This suggests that errors of an order of magnitude are not unusual. A more detailed statistical treatment of 490 values relating mainly to reaction rate constants k_r is given in Appendix II where attempts are made to obtain better values by taking proper account of the fact that many of the bimolecular rate constants have been measured relative to the bimolecular rate constants of other substrates or standards, and the choice of the values for such standards affects many other values and thereby the average values for k_r for many compounds. From the statistical treatment which includes almost 500 measurements on 59 compounds in about 40 different solvents, it is concluded that the 95% confidence limit is a factor of 12.7 for two measurements and only compounds with seven or more measurements have 95% confidence limits of less than a factor of two (see table A3 in Appendix II for full details). Only in the extreme case of 1,3-diphenylisobenzofuran, entry 5.36, (assuming solvent effects are negligible, see Appendix II) is the 95% confidence limit obtained from 104 values better than the expected uncertainty of individual measurements claimed by authors and as low as 14%. The question of solvent effects on the bimolecular rate constants is fully discussed in Appendix II. Since Appendix II treats statistically most of the results which have been measured many times by the same and different authors, estimates of errors for values of k, k_r and k_q not included in this treatment may be taken as having similar large uncertainties and unfortunately only when many measurements, e.g. more than seven, have been made can one expect 95% confidence limits less than a factor of two.

6.1. Mechanisms of Quenching

As indicated earlier, quenching of singlet oxygen may be due to chemical reaction or physical quenching. Physical quenching of singlet oxygen has been established as due to electronic energy transfer [46] and as a result of favourable charge-transfer interaction [67,68,69]. For diamagnetic substrates electronic energy transfer is possible whenever the energy of the lowest excited triplet state of a quencher lies below that of singlet oxygen. Thus the occurrence of the spin allowed process

$$^1O_2^* + {}^1Q \rightarrow {}^3Q^* + {}^3O_2$$

has been confirmed in the case of β-carotene and other polyenes with low lying triplet states [46,48]. Electronic energy transfer has also been proposed to account for the highly efficient quenching by certain dyes [43,70] and by several coordination complexes [46] (see table 10).

Physical quenching resulting from favorable charge-transfer interactions was first demonstrated with various amines [67-69]. Thus Young et al. [71], have shown that for a series of *N,N*-dimethylanilines a Hammett plot can be drawn with a ρ value of -1.39 which supports the suggestion that a complex which is charge transfer in nature is responsible for this type of quenching which may be

represented as follows:

$$^1O_2^* + NR_3 \rightleftarrows {}^1(O^{\delta-}...NR^{\delta+}) \rightleftarrows {}^3(O^{\delta-}...NR^{\delta+}) \rightarrow {}^3O_2 + NR_3.$$

In agreement with this scheme the lower the ionization potential of the amine the better it is as a quencher. Thus quenching rate constants are in the order tertiary > secondary > primary amines (see table 6). However, even the most efficient charge–transfer quenchers such as DABCO (entry 6.40) have quenching rate constants about two orders of magnitude less than diffusion controlled. It is of interest to note that the efficiency of quenching by amines in the gas phase is similar to that observed in solution [67,68,69] which is in keeping with the lack of any large solvent effect [see tables 6 and 7].

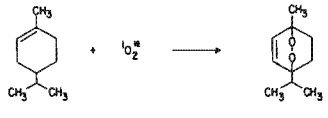
Physical quenching due to electronic to vibronic energy transfer has already been mentioned in section 5 where the dependence of the lifetime on high energy vibrations in the solvent was discussed. There is little evidence for a heavy-atom enhancement of the intersystem crossing from singlet to triplet O_2, neither does quenching by paramagnetic species, which could arise from the catalysed intersystem crossing process

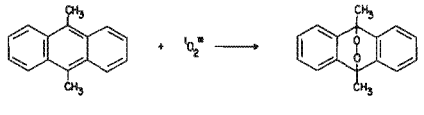
$$^1O_2^* + {}^mQ \rightarrow {}^3O_2 + {}^mQ$$

which is spin allowed by Wigners Spin rule, give rise to efficient quenching since for example $k_q \leq 10^4$ dm^3 mol^{-1} s^{-1} for quenching of $^1O_2^*$ by $^3O_2$ (see entry 15.1) (see [72] for further discussion of physical quenching of singlet oxygen).

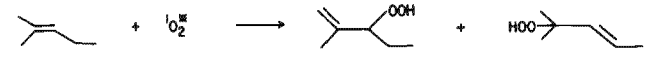
Chemical reactions of singlet oxygen have been discussed in detail in a number of reviews e.g. [9,30–37]. The primary products, formed from $^1O_2^*$ reactions with hydrocarbons and many substituted hydrocarbons containing one or more double bonds are often of variable stability, but they appear to be formed in only three types of reaction

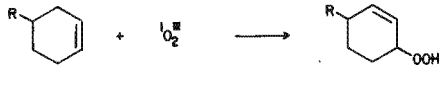
(i) formation of endoperoxides, e.g.



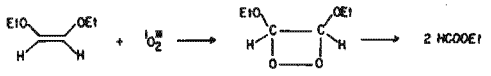


(ii) formation of allyl hydroperoxides, by 'ene' reactions e.g.



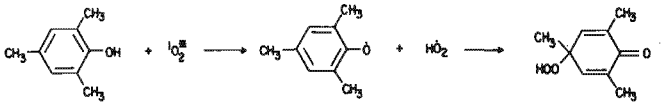


(iii) formation of 1,2–dioxetanes



Various reducing agents also react quite efficiently with singlet oxygen, viz.

(iv)



(v) $Et_2S + {}^1O_2^* \rightarrow Et_2SOO\ (+ Et_2S) \rightarrow 2Et_2SO$

(vi) $CH_3CH_2NH_2 + {}^1O_2^* \rightarrow CH_3CH(OOH)NH_2.$

An examination of the data in this compilation makes the authors suggest that there is a great need for further careful work to establish more precise values, especially for those compounds which are in effect being used as standards. If such measurements can be made independently at more than one laboratory with a proper treatment of errors, so much the better.

It is hoped that the compilation will be updated periodically and it is hoped readers will bring to our attention any new results, any results inadvertently missed from our literature searches, and any noted errors.

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Abbreviations

General

S	sensitizer
A	primary substrate
A′	reference substrate
A″	second reference substrate
P	product of primary substrate
P′	product of reference substrate
$^1O_2$*	singlet oxygen

Sensitizers

An	anthracene
azine	3*H*–2–pivaloyl–4–phenyl–6–diethylamino–8–methylquinoxal–3–one
BA	1,2–benzanthracene
BP	benzophenone
DMA	9,10–dimethylanthracene
DNT	dinaphthalene thiophene
Eos	eosin
Ery	erythrosine
FMN	riboflavin–5′–phosphate (flavine mononucleotide)
MB	methylene blue
MP	*meso*–porphyrin
Naph	naphthalene
Per	perylene
Phen	phenanthrene
PP	protoporphyrin
Py	pyrene
RB	rose bengal
RBCE	rose bengal complexed with dicyclohexyl–18–crown–6
Rub	rubrene
self	self sensitization
Tetr	tetracene
TPP	tetraphenylporphine
ZnTPP	zinc tetraphenylporphine

Reference substrates

Car	all *trans*–β–carotene
DABCO	1,4–diazabicyclooctane
p–dioxene	3,6–dioxacyclohexene
DDM	diazodiphenylmethane
DMA	9,10–dimethylanthracene
DMBA	9,10–dimethyl–1,2–benzanthracene
DPBF	1,3–diphenylisobenzofuran
DPF	2,5–diphenylfuran
Rub	rubrene
TMS	trimethylstyrene
2M2B	2–methyl–2–butene
TME	2,3–dimethyl–2–butene (tetramethylethylene)
2M2P	2–methyl–2–pentene
TMHP	2,2,6,6–tetramethyl–4–hydroxypiperidine

Substrate column

TBA	tetrabutylammonium ion
TOS	*p*–toluenesulfonate ion

Chemical groups

Me–	CH_3
Et–	CH_2CH_3
n–Pr–	$CH_2CH_2CH_3$
i–Pr–	$CH(CH_3)_2$
n–Bu–	$CH_2(CH_2)_2CH_3$
s–Bu–	$CH(CH_3)CH_2CH_3$
t–Bu–	$C(CH_3)_3$
Ph–	C_6H_5
dtc	dithiocarbamate
acac	acetylacetonate

Solvent column

(5:1) v:v	5 parts to 1 part by volume
i–octane	2,2,4–trimethylpentane
THF	tetrahydrofuran

Rate data columns

k_r^A	rate constant for chemical reaction of A
β_r^A	beta value for chemical reaction of A
k_q^A	rate constant for physical quenching of $^1O_2$*
β_q^A	beta value for physical quenching of $^1O_2$*
k	rate constant including both k_r^A and k_q^A components
β	beta value including both β_r^A and β_q^A components
k_d	rate constant for solvent deactivation
k_D	$(k_d + k_A[A])$
k_{Td}^A	rate constant for substrate quenching of sensitizer triplets
(est)	estimated from an experimentally determined quantity

Temperature column

rt	temperature not reported, possibly room temperature

Methods column

Od–	rate monitored by oxygen disappearance
Ad–	rate monitored by substrate disappearance
A′d–	rate monitored by reference substrate disappearance
Pa–	rate monitored by product appearance
P′a–	rate monitored by reference product appearance
Ld–	rate monitored by $^1O_2$* luminescence decay

Comments column

SDS	sodium dodecyl sulfate
DTAC	dodecyltrimethylammonium chloride
CTAB	hexadecyltrimethylammonium bromide
$[A]_0$	initial concentration of A
calc	calculated
decomp.	decomposition
r_{ox}	reaction rate of oxidation
Φ_{isc}	quantum yield of sensitizer triplet state production
E_a	Activation energy for rate constant k.

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TABLE 1. Decay constants of singlet oxygen in various solvents

No.	Solvent	k_d/s^{-1}	t/°C	Comments	Ref.
1.1	H_2O (water)	‡$(5.0 \pm 2.0) \times 10^5$	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d extrapolated from a value in (H_2O/MeOH) (1:1) v:v mixture.	Merk.72F026
1.1.1		‡4.8×10^5	rt	S = MB, A = DPBF, dye laser (610 nm). k_d corrected to zero MeOH concentration.	Youn.76F903
1.1.2		‡3.3×10^5	rt	S = 2-acetonaphthone, A = DPBF, nitrogen laser (337 nm).DPBF solubilized in SDS micelles in air saturated H_2O solutions.	Gorm.78E144
1.1.3	k_d(Av) =	*4.4×10^5			
1.2	D_2O (water-d_2)	‡$(3.0 \pm 0.2) \times 10^4$	20	S = MB, A = DPBF, dye laser (620 nm). k_d determined in air saturated D_2O solutions of DPBF solubilized in SDS micelles.	Math..78E143
1.2.1		‡$(2.8 \pm 0.2) \times 10^4$	20	S = MB, A = DPBF, dye laser (620 nm). k_d determined in air saturated D_2O solutions of DPBF solubilized in CTAB micelles.	Math..78E143
1.2.2		‡3.3×10^4	rt	S = 2-acetonaphthone, A = DPBF, nitrogen laser (337 nm). DPBF solubilized in SDS micelles in air saturated D_2O solutions.	Gorm.78E144
1.2.3	k_d(Av) =	*3.1×10^4			
1.3	CH_3OH (methanol)	$(1.4 \pm 0.2) \times 10^5$	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.71M325
1.3.1		<$(2.0 \pm 0.2) \times 10^5$	23	S = MB,BP,Naph,An,Phen,BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_r[DPBF] contribution. For revised value see [76F902]. Error is a standard deviation.	Adam.72F126
1.3.2		‡$(8.8 \pm 0.4) \times 10^4$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
1.3.3		‡$(9.7 \pm 1.1) \times 10^4$	rt	S = RB, A = DPBF, dye laser (583 nm). Error is a 95% confidence limit.	Youn..73F014
1.3.4		‡$(1.1 \pm 0.2) \times 10^5$	rt	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
1.3.5		‡1.1×10^5	25	S = MB, A = DPBF, ruby laser (694 nm).	Usui..78F061
1.3.6	k_d(Av) =	*$(1.0 \pm 0.2) \times 10^5$			
1.4	CH_2Cl_2 (dichloromethane)	‡1.6×10^4	25	S = MB, A = DPBF, ruby laser (694 nm).	Usui..78F061
1.4.1		‡7.1×10^3	rt	S = MB, A = DPBF, dye laser (610 nm).	Youn.76F903
1.4.2	k_d(Av) =	*1.2×10^4			
1.5	$CHCl_3$ (chloroform)	‡$(1.7 \pm 0.4) \times 10^4$	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d decreases by 50 % on lowering the temperature from 25 °C to -50 °C.	Long.75F088
1.5.1		‡$(4.4 \pm 1.8) \times 10^3$	rt	S = MB, A = DPBF, dye laser (610 nm).	Youn.76F903
1.5.2		‡9.0×10^3	25	S = MB, A = DPBF, ruby laser (694 nm).	Usui..78F061
1.5.3	k_d(Av) =	*1.0×10^4			
1.6	$CDCl_3$ (chloroform-d)	$(3.3 \pm 1.0) \times 10^3$	rt	S = MB, A = DPBF, ruby laser (694 nm).	Long.75F088
1.7	CF_3Cl (Freon-11)	$(1.0 \pm 0.2) \times 10^3$	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d corrected for 1-2% MeOH content.	Long.75F088
1.8	CCl_4 (carbon tetrachloride)	‡$(1.4 \pm 0.7) \times 10^3$	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d corrected for 2% MeOH content.	Merk.72F260
1.8.1		‡2.2×10^3	rt	S = MB, A = DPBF, dye laser (610 nm).	Youn.76F903
1.8.2		‡$(1.42 \pm 0.40) \times 10^3$	25	S = MB, A = DPBF, flash photolysis. k_d from extrapolation to zero [MeOH] using k_d values for CCl_4/MeOH mixtures (1-5% MeOH).	Furu.78E238
1.8.3		**3.6×10^1	rt	S = TPP,PP,MP,pheophytins. k_d from direct measure of decay of sensitized luminescence from $^1O_2$* using a phosphoroscope.	Kras79A010
1.8.4	k_d(Av) =	*1.7×10^3			
1.9	CS_2 (carbon disulfide)	$(5.0 \pm 1.5) \times 10^3$	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d corrected for 1% MeOH content.	Merk.72F260
1.10	CH_3CH_2OH (ethanol)	‡$(8.3 \pm 1.7) \times 10^4$	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F260
1.10.1		‡$(1.0 \pm 0.1) \times 10^5$	rt	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902

TABLE 1. Decay constants of singlet oxygen in various solvents — Continued

No.	Solvent	k_d/s^{-1}	$t/°C$	Comments	Ref.
1.10.2		‡(5.3 ± 0.9) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.10.3	k_d(Av) =	*7.9 x 10^4			
1.11	$HO(CH_2)_2OH$ (1,2-dihydroxy-ethane)	4.8 x 10^5	rt	S = MB or RB, A = DPBF, dye laser. k_D = 5.1 x 10^5 s^{-1} when [DPBF] = 1.7 x 10^{-5} mol dm^{-3} and β = 3.2 x 10^{-4} mol dm^{-3} (for method see section (4)).	Youn.73F014
1.11.1		*1.6 x 10^5	rt	S = MB, A = DPBF, dye laser (610 nm). k_d corrected to zero MeOH concentration. k_d value very different from previous value of same authors [73F014].	Youn.76F903
1.12	CH_2FCH_2OH (2-fluoroethanol)	(5.6 ± 1.2) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.13	CH_3CHCl_2 (1,1-dichloroethane)	1.5 x 10^4	25	S = MB, A = DPBF, ruby laser (694 nm).	Usui.:78F061
1.14	$CHCl_2CH_2OH$ (2,2-dichloro-ethanol)	(2.1 ± 0.6) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.15	CCl_3CH_2OH (2,2,2-trichloro-ethanol)	(2.0 ± 0.6) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.16	CF_3CH_2OH (2,2,2-trifluoro-ethanol)	(2.3 ± 0.6) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.17	CH_3CN (acetonitrile)	‡(3.3 ± 0.7) x 10^4	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F260
1.17.1		‡(1.8 ± 0.3) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90 % confidence limit.	Youn.76F903
1.17.2	k_d(Av) =	*2.55 x 10^4			
1.18	$CHCl_2CHCl_2$ (1,1,2,2-tetra-chloroethane)	8.3 x 10^3	25	S = MB, A = DPBF, ruby laser (694 nm).	Usui..78F061
1.19	$CH_3CHOHCH_3$ (2-propanol)	(5.0 ± 0.3) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.20	$CH_3(CH_2)_2Br$ (1-bromopropane)	‡(1.0 ± 0.2) x 10^5	rt	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
1.20.1		‡(1.3 ± 0.4) x 10^5	rt	S = An, Q = Car, ruby laser (347 nm). k_d measured by following the disappearance of triplet β-carotene. (See section 2.2)	Wilk76F902
1.20.2	k_d(Av) =	*1.15 x 10^5			
1.21	$HCON(CH_3)_2$ (dimethyl-formamide)	⩽(1.4 ± 0.1) x 10^5	23	S = An,Phen,Py,BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_d[DPBF] contribution. Error is a standard deviation.	Adam.72F126
1.22	CH_3COCH_3 (acetone)	‡(3.8 ± 0.8) x 10^4	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F026
1.22.1		‡(2.4 ± 0.5) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.22.2	k_d(Av) =	*3.1 x 10^4			
1.23	CH_2OCHCH_2Br (1-bromo-2,3-epoxy-propane)	(2.2 ± 0.5) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.24	$CH_3(CH_2)_3OH$ (1-butanol)	(5.2 ± 0.8) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
1.25	$(CH_3)_3COH$ (2-methyl-2-propanol)	(3.0 ± 0.4) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
1.26	C_4H_8O (tetrahydrofuran)	(4.3 ± 0.4) x 10^4	rt	S = RB, A = DPBF, dye laser (583 nm). Error is a 90% confidence limit.	Youn.76F903
1.27	$C_4H_8O_2$ (dioxane)	(2.9 ± 1.0) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
1.28	$CH_3COOCH_2CH_3$ (ethyl acetate)	(2.1 ± 0.7) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.29	C_5H_5N (pyridine)	(3.1 ± 1.4) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn.73F014

TABLE 1. Decay constants of singlet oxygen in various solvents — Continued

No.	Solvent	k_d/s^{-1}	$t/°C$	Comments	Ref.
1.29.1		*(5.9 ± 1.4) x 10^4	rt	S = RB, A = DPBF, dye laser (583 nm). k_d value very different from previous one by same authors [73F014]. Error is a 90% confidence limit.	Youn.76F903
1.30	C_6H_{12} (cyclohexane)	(5.9 ± 0.2) x 10^4	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d corrected for 2% MeOH content.	Merk.72F260
1.31	$C_6H_{11}OH$ (cyclohexanol)	(6.3 ± 0.9) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.32	C_6H_6 (benzene)	‡(4.2 ± 0.9) x 10^4	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F026
1.32.1		<(8.0 ± 0.5) x 10^4	23	S = Naph,BP,An,Phen,Py,BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_r[DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation.	Adam.72F126
1.32.2		<(7.0 ± 1.0) x 10^4	23	S = BA, A = DPBF, ruby laser (347 nm). Value not corrected for k_r[DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation.	Adam.72F126
1.32.3		<(8.0 ± 2.0) x 10^4	5	S = BA, A = DPBF, ruby laser (347 nm). Value not corrected for k_r[DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation.	Adam.72F126
1.32.4		‡(3.9 ± 0.4) x 10^4	rt	S = An, A = DPBF, ruby laser (347 nm).	Farm.73F438
1.32.5		‡(4.1 ± 0.3) x 10^4	rt	S = An, Q = Car, ruby laser (347 nm). k_d measured by following the disappearance of triplet β-carotene. (See section 2.2)	Farm.73F438
1.32.6		‡(3.7 ± 0.6) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.32.7		‡3.7 x 10^4	rt	S = Tetr, A' = DPBF. Sensitizer excited with pulsed electron beam (0.5-10 krad). k_d from extrapolation to zero dose of electrons.	Gorm..78E263
1.32.8		‡(4.1 ± 0.4) x 10^4	rt	S = An, Q = Car, ruby laser (347 nm). k_d measured by following the disappearance of triplet β-carotene. (See section 2.2)	Wilk.78F276
1.32.9	k_d(Av) =	*(4.0 ± 0.7) x 10^4			
1.33	C_6D_6 (benzene-d_6)	(2.8 ± 0.6) x 10^4	rt	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
1.34	C_6H_5Br (bromobenzene)	(1.3 ± 0.6) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.35	C_6F_6 (hexafluoro-benzene)	(1.7 ± 0.6) x 10^3	rt	S = MB, A = DPBF, ruby laser (694 nm). k_d corrected for 1-2% MeOH content.	Long.75F088
1.36	$C_6H_5CH_3$ (toluene)	4.0 x 10^4	rt	S = Tetr, A' = DPBF. Sensitizer excited with pulsed electron beam (0.5-10 krad). k_d from extrapolation to zero dose of electrons.	Gorm..78E263
1.37	$C_6H_5COOCH_3$ (methyl benzoate)	(2.5 ± 1.0) x 10^4	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Youn.76F903
1.38	H_2O/CH_3OH (1:1) v:v	‡2.9 x 10^5	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F027
1.38.1		‡(2.8 ± 0.8) x 10^5	rt	S = MB or RB, A = DPBF, dye laser. k_D = 3.7 x 10^5 s^{-1} when [DPBF] = 1.7 x 10^{-5} mol dm^{-3} and β = 5.5 x 10^{-5} mol dm^{-3} (for method see section (5)).	Youn..73F014
1.38.2	k_d(Av) =	*2.9 x 10^5			
1.39	D_2O/CH_3OH (1:1) v:v	9.1 x 10^4	rt	S = MB, A = DPBF, ruby laser (694 nm).	Merk.72F027
1.40	CH_3OH /$HO(CH_2)_2OH$ (1:1) v:v	(1.2 ± 0.2) x 10^5	rt	S = MB or RB, A = DPBF, dye laser. k_D = 1.6 x 10^5 s^{-1} when [DPBF] = 1.9 x 10^{-5} mol dm^{-3} and β = 6.3 x 10^{-5} mol dm^{-3} (for method see section (5)).	Youn..73F014
1.41	CCl_4/CH_3OH (99:1) v:v	(3.0 ± 2.0) x 10^3	25	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Brew74F646

TABLE 1. Decay constants of singlet oxygen in various solvents — Continued

No.	Solvent	k_d/s^{-1}	t/°C	Comments	Ref.
1.42	CCl_4/CH_3OH (98:2) v:v	$(3.2 \pm 0.5) \times 10^3$	25	S = MB, A = DPBF, flash photolysis.	Furu.78E238
1.43	CCl_4/CH_3OH (94.3:5.7) v:v	$(5.0 \pm 1.0) \times 10^3$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Brew74F646
1.44	CCl_4/CH_3OH (90.1:9.9) v:v	$(9.0 \pm 4.0) \times 10^3$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Brew74F646
1.45	CCl_4/CH_3OH (86.2:13.8) v:v	$(1.1 \pm 0.3) \times 10^4$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Brew74F646
1.46	CCl_4/CH_3OH (82.7:17.3) v:v	$(1.5 \pm 0.2) \times 10^4$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit.	Brew74F646
1.47	CS_2/MeOH (98:2) v:v	$(4.0 \pm 0.4) \times 10^3$	rt	S = MB, A = DPBF, flash photolysis.	Floo..73F334
1.48	CH_3CH_2OH/H_2O (95:5) v:v	$< (1.8 \pm 0.2) \times 10^5$	23	S = Naph,An,Phen,Py,BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_r[DPBF] contribution. For revised value see [76F9O2]. Reported error is a standard deviation.	Adam.72F126
1.48.1		$<(1.3 \pm 0.2) \times 10^5$	23	S = MB, A = DPBF, ruby laser (347 nm). Value not corrected for k_r[DPBF] contribution. For revised value see [76F902]. Reported error is a standard deviation.	Adam.72F126
1.48.2		$<(1.3 \pm 0.1) \times 10^5$	0	S = MB, A = DPBF, ruby laser (347 nm). Value not corrected for k_r[DPBF] contribution. For revised value see [76F902]. Reported error is a standard deviation.	Adam.72F126
1.48.3		$*(2.0 \pm 0.8) \times 10^5$	rt	S = An, Q = Car, ruby laser (347 nm). k_d measured by following the disappearance of triplet β-carotene. (See section 2.2)	Wilk76F902
1.49	C_6H_6/CH_3OH (4:1) v:v	$(3.8 \pm 0.8) \times 10^4$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
1.50	C_6H_5Br/CH_3OH (4:1) v:v	$(4.3 \pm 0.7) \times 10^4$	rt	S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014

‡ These values of k_d are averaged to obtain the preferred value of k_d labeled with an *.

* Preferred value of k_d used to convert β values in tables 2 thru 15.

** See text section (5) for a discussion of this value.

TABLE 1(a). *Decay constants of singlet oxygen in various solvents; estimates from indirect methods where no value is available from direct methods*

No.	Solvent	k_d/s^{-1}	$t/°C$	Comments	Ref.
1(a).0	CH_3CH_2I	2.5×10^5 (est)	rt	k_d estimated using eq. (39) from text and $k_A(CH_3CH_2I) = 4 \times 10^6$ dm^3 mol^{-1} s^{-1} [*15.4*].	Wilk76F902
1(a).1	$(CH_3)_2SO$ (dimethylsulfoxide)	5.2×10^4 *3.4×10^4 (est)	rt	S = RB, A = DPBF, A′ = 2M2P. Measured $\beta_{A'} = (5.5 \pm 0.1) \times 10^{-2}$ mol dm^{-3}, assumed $k_{A'} = 9.38 \times 10^5$ (*6.25×10^5) dm^3 mol^{-1} s^{-1} (value in MeOH from [*2.40.2*]).	Guir.76E072
1(a).1.1		3.33×10^4 (est)	rt	Method not reported, may be direct method given in ref. [71M325].	Nils.74F643
1(a).2	CCl_2FCClF_2 (Freon-113)	4.3×10^2 (est)	rt	A = Rub. k_d estimated from β_A(Freon-113) = 1.1×10^{-5} mol dm^{-3} assuming $k_A = 3.9 \times 10^7$ dm^3 mol^{-1} s^{-1} where k_A is an average of all values listed under entry *3.63*.	Stev76F905
1(a).2.1		5.0×10^2 (est)	rt	A = DPBF. k_d estimated from β_A(Freon-113) = 5.4×10^{-7} mol dm^{-3} assuming $k_A = 9.2 \times 10^8$ dm^3 mol^{-1} s^{-1} where k_A is an average of all values listed under entry *5.36*.	Stev76F905
1(a).3	$(CD_3)_2CO$ (acetone-d_6)	3.8×10^4 *3.1×10^4 (est)	rt	S = MB, A = Rub. Measured r_{ox} in $(CH_3)_2CO$ and $(CD_3)_2CO$ to be identical. Assumed k_A to be independent of solvent composition. Took $k_d((CH_3)_2CO) = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Merk.72F260
1(a).4	$CH_3(CH_2)_3O(CH_2)_2OH$ (2-butoxyethanol)	3.8×10^5 (est)	0	A = Rub, Q = DABCO, $^1O_2$* from microwave discharge. Assumed $k_Q = 3.4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_A = 7.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and used equation (33).	Carl...72F319
1(a).5	C_6H_5Cl (chlorobenzene)	1.6×10^4 (est)	25	S = TPP, A = 3-methyl-2-pentene. The authors assumed $k_A = 1.0 \times 10^6$ dm^3 mol^{-1} s^{-1}. However they give $\beta_A = 1.64 \times 10^{-2}$ mol dm^{-3} in the text and $\beta_A = 1.6 \times 10^{-4}$ mol dm^{-3} in a table. Using these values with k_A gives estimates for k_d of 1.6×10^4 s^{-1} and 1.6×10^2 s^{-1} respectively.	Carl..74F341
1(a).6	$(CH_3)_2CHCH_2C(CH_3)_3$ (2,2,4-trimethylpentane) (*i*-octane)	4.0×10^4 (est)	25	S = A = Rub, Q = DABCO. Assumed $k_Q = 3.4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and used equation (23).	Carl...72F319
1(a).6.1		4.7×10^4 (est)	25	A = Rub, $^1O_2$* from $(PhO)_3PO_3$ decomp. Measured $\beta_A = 6.4 \times 10^{-4}$ mol dm^{-3}, assumed $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}. Solvent contained 5% by volume of both MeOH and C_5H_5N.	Carl..74F341
1(a).7	$CH_3(CH_2)_{14}CH_3$ (hexadecane)	9.0×10^4 (est)	25	A = Rub, $^1O_2$* from microwave discharge. Measured $\beta_A = 1.2 \times 10^{-3}$ mol dm^{-3}, assumed $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and used equation (33).	Carl..74F341
1(a).8	D_2O/CD_3OD (1:1) v:v	2.9×10^4 (est)	rt	S = MB, A = DPBF. Measured r_{ox} in both H_2O/CH_3OH and D_2O/CD_3OD. Assumed k_A is insensitive to solvent composition and $k_d(H_2O/CH_3OH) = (2.9 \pm 0.5) \times 10^5$ s^{-1} [*1.38.2*].	Merk..72F027
1(a).9	CH_2Cl_2/CH_3OH (11:5) v:v	2.1×10^4 (est)	rt	A = Rub, Q = *cis*- and *trans*-1,4-dicloro-1,4-dinitrosocyclohexane, $^1O_2$* from $(PhO)_3PO_3$ decomp. Assumed $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Sing.76F900
1(a).10	CH_2Cl_2/CH_3OH (15:1) v:v	1.1×10^4 (est)	rt	A = Rub, Q = $(CH_3)_3CNO$, $^1O_2$* from $(PhO)_3PO_3$ decomp. Assumed $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Sing.76F900
1(a).11	$CH_2Cl_2/C_5H_5N/MeOH$ (93:3:3) v:v:v	5.0×10^4 (est)	25	A = Rub, Q = DABCO, $^1O_2$* from $(PhO)_3PO_3$ decomp. Measured β_A = (unreported), assumed $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and used equation (30).	Carl...72F319

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
2.1	ethoxyethene $CH_2=CHOC_2H_5$	$(Me)_2CO$	$k_r = 5.7 \times 10^4$ *4.7×10^4		8	?	S = ? A′ = *p*-dioxene. Measured $(k_r/k_r^{A'})$ = 0.26. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
2.1.1		$(Me)_2CO$	4.3×10^4 *3.5×10^4	$(8.8 \pm 0.2) \times 10^{-1}$	15	A′d–16	S = RB, A′ = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.1.2		$(Me)_2CO$	$k_r = 3.1 \times 10^4$ *2.5×10^4		6	Ad–17 A′d	S = RB, A′ = *p*-dioxene. Measured $(k_r/k_r^{A'})$ = 0.14 ± 0.03. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*]. Found $k_r >> k_q$.	Fale77F876
2.1.3		C_6H_6	2.3×10^5	$(1.8 \pm 0.1) \times 10^{-1}$	15	A′d–16	S = RBCE, A′ = DPBF. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Fale77F876
2.2	1,1-diethoxyethene $CH_2=C(OC_2H_5)_2$	$(Me)_2CO$	4.6×10^5 *3.7×10^5	$(8.3 \pm 0.2) \times 10^{-2}$	15	A′d–16	S = RB, A′ = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.2.1		$(Me)_2CO$	$k_r < 1 \times 10^4$ (est)		6	Ad–17 A′d	S = RB, A′ = *p*-dioxene. No measurable reaction of A.	Fale77F876
2.2.2		C_6H_6	2.6×10^5	$(1.5 \pm 0.1) \times 10^{-1}$	15	A′d–16	S = RBCE, A′ = DPBF. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Fale77F876
2.3	*cis*-1,2-diethoxy-ethene $C_2H_5OCH=CHOC_2H_5$	$(Me)_2CO$	$k_r = 3.3 \times 10^7$ *2.7×10^7		8	?	S = ?, A′ = *p*-dioxene. Measured $(k_r/k_r^{A'})$ = 151. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5)dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
2.3.1		$(Me)_2CO$	4.4×10^7 *3.6×10^7	$(8.6 \pm 0.1) \times 10^{-4}$	15	A′d–16	S = RB, A′ = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.3.2		$(Me)_2CO$	$k_r = 5.7 \times 10^7$ *3.2×10^7		6	Ad–17 A′d	S = RB, A′ = TME. Measured $(k_r/k_r^{A'})$ = 1.06. k_r derived using $k_r^{A'} = 5.4 \times 10^7$ (*3.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.2*]. Found $k_r >> k_q$.	Fale77F876
		For more relative rates see 2.4.2.						
2.4	*trans*-1,2-diethoxy-ethene $C_2H_5OCH=CHOC_2H_5$	$(Me)_2CO$	$k_r = 1.0 \times 10^7$ *8.3×10^6		8	?	S = ?, A′ = *p*-dioxene. Measured $(k_r/k_r^{A'})$ = 46. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
2.4.1		$(Me)_2CO$	4.7×10^7 *3.8×10^7	$(8.13 \pm .02) \times 10^{-4}$	15	A′d–16	S = RB, A′ = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

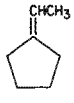
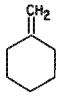
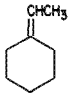
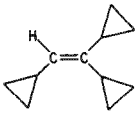
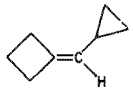
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.4.2		$(Me)_2CO$	$k_r = 2.6 \times 10^7$ *1.5×10^7		6	Ad–17 A′d	S = RB, A′ = *cis*–1,2–diethoxyethene. Measured $(k_r/k_r^{A'}) = 4.55 \times 10^{-1}$. k_r derived using $k_r^{A'} = 5.7 \times 10^7$ (*3.2×10^7) dm^3 mol^{-1} s^{-1} [*2.3.2*].	Fale77F876
2.5	methylidene–cyclopentane 	CH_3CN	$k_r = 4.6 \times 10^4$		rt	?	S = MB, A′ = 1–methylcyclohexene. Measured $(k_r/k_r^{A'}) = 0.23$. k_r derived using $k_r^{A'} =$ *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.5.1		CH_3CN	$k_r = 5.6 \times 10^4$		0	Ad–17 A′d	S = MB, A′ = 2–methylidenenorborn–5–ene. Measured $(k_r/k_r^{A'}) = 15.5$. k_r derived using $k_r^{A'} = 3.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.94b*].	Jeff..78F149
2.6	ethylidene–cyclopentane 	$CHCl_3$	$(8.7 \pm 1.3) \times 10^6$		rt	A′d–33	S = A′ = Rub. k derived using $k_{A\cdot} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
2.7	methylidene–cyclohexane 	CH_3CN	$k_r < 1 \times 10^3$ (est)		rt	?	S = MB, A′ = 1–methylcyclohexene.	Jeff....73F664
2.8	ethylidene–cyclohexane 	$CHCl_3$	$(8.6 \pm 1.3) \times 10^5$		rt	A′d–33	S = A′ = Rub. k derived using $k_{A\cdot} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
2.9	1,1,2–triethoxyethene $C_2H_5OCH{=}C(OC_2H_5)_2$	$(Me)_2CO$	1.2×10^8 *1.0×10^8	$(3.07 \pm .06) \times 10^{-4}$	15	A′d–16	S = RB, A′ = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.10	1,1,2–tricyclopropylethene 	$(Me)_2CO$	$k_r = 5.2 \times 10^5$		rt	Ad–17 A′d	S = Eos, A′ = (dicyclopropylmethylidene)–cyclobutane. Measured $(k_r/k_r^{A'}) = 0.40$. k_r derived using $k_r^{A'} =$ 1.3×10^6 dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430
2.11	(cyclopropylmethylidene)cyclobutane 	$(Me)_2CO$	$k_r = 7.7 \times 10^5$		rt	Ad–17 A′d	S = Eos, A′ = (dicyclopropylmethylidene)cyclobutane. Measured $(k_r/k_r^{A'}) = 0.59$. k_r derived using $k_r^{A'} =$ 1.3×10^6 dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

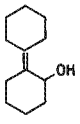
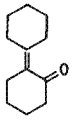
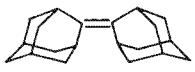
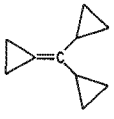
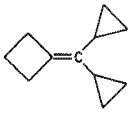
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.12	1,1,2,2-tetra-ethoxyethene $(C_2H_5O)_2C=C(OC_2H_5)_2$	$CHCl_3$	7.6×10^7 *4.5×10^7	$(2.2 \pm 0.2) \times 10^{-4}$	15	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 1.7 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*]. Solvent contained 1% EtOH.	Fale77F876
2.12.1		CH_3CN	4.3×10^7 *3.3×10^7	$(7.69 \pm .04) \times 10^{-4}$	15	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*].	Fale77F876
2.12.2		$(Me)_2CO$	4.5×10^7 *3.6×10^7	$(8.5 \pm 0.1) \times 10^{-4}$	15	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.12.3		$(Me)_2CO$	$k_r = 4.6 \times 10^7$ *2.6×10^7		6	Ad-17 A'd	S = RB, A' = TME. Measured ($k_r/k_r^{A'}$) = 0.854. k_r derived using $k_r^{A'} = 5.4 \times 10^7$ (*3.0×10^7) dm^3 mol^{-1} s^{-1} [*43.2*]. Found $k_r >> k_q$.	Fale77F876
2.12.4		C_6H_6	7.4×10^7	$(5.67 \pm .18) \times 10^{-4}$	15	A'd-16	S = RBCE, A' = DPBF. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Fale77F876
2.13	cyclohexylidene-cyclohexane 	MeOH(?)	1.8×10^6	5.6×10^{-2}	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.13.1		MeOH	3.3×10^6	3.0×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 5.4 kJ mol^{-1}.	Koch68F288
2.14	2-cyclohexyl-idene-cyclohexanol 	MeOH(?)	2.3×10^5	4.4×10^{-1}	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.15	2-cyclohexyl-idene-cyclohexanone 	MeOH(?)	2.7×10^5	3.7×10^{-1}	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.15.1		MeOH	2.9×10^5	3.5×10^{-1}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 11.7 kJ mol^{-1}.	Koch68F288
2.16	$\Delta^{9,10}$-octalin 	$CHCl_3$	$(5.0 \pm 0.8) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.17	adamantylidene-adamantane(2) 	$CHCl_3$	1.02×10^6 *6.13×10^5	1.63×10^{-2}	15	A'd-16	S = MB, A' = DPBF. k derived using k_d = 1.7×10^4 (*1.0×10^4) s^{-1} [*1.5*]. Solvent contained 1% EtOH.	Fale77F876
2.18	(dicyclopropylmethylidene)cyclopropane 	$(Me)_2CO$	$k_r = 1.4 \times 10^6$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured ($k_r/k_r^{A'}$) = 1.05. k_r derived using $k_r^{A'}$ = 1.3×10^6 dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430
2.19	(dicyclopropylmethylidene)cyclobutane 	MeOH	$k_r = 1.1 \times 10^6$		rt	Ad-17 A'd	S = Eos, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.1 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430
2.19.1		CH_2Cl_2	$k_r = 1.1 \times 10^6$		rt	Ad-17 A'd	S = MB, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.1 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430
2.19.2		CS_2	$k_r = 1.1 \times 10^6$		rt	Ad-17 A'd	S = TPP, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.2 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430
2.19.3		CH_3CH_2I	$k_r = 1.1 \times 10^6$		rt	Ad-17 A'd	S = TPP, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.1 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430
2.19.4		$(Me)_2CO$	$k_r = 1.3 \times 10^6$		rt	Ad-17 A'd	S = Eos, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.6 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430
2.19.5		C_6H_6	$k_r = 1.3 \times 10^6$		rt	Ad-17 A'd	S = TPP, A' = TMS. Measured ($k_r/k_r^{A'}$) = $(2.5 \pm 0.4) \times 10^{-1}$. k_r derived using $k_r^{A'}$ = 5.0×10^6 dm^3 mol^{-1} s^{-1} [*3.10*].	Rous..78F430

For more relative rates see 2.10, 2.11, 2.18, 2.20 2.23, 2.24, 2.25, 2.27, 2.34, 2.36, 3.20

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

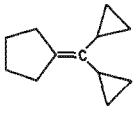
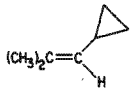
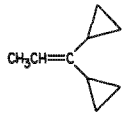
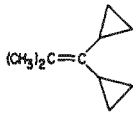
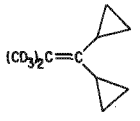
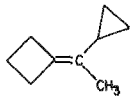
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.20	(dicyclopropylmethylidene)cyclopentane 	$(Me)_2CO$	$k_r = 1.2 \times 10^6$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)cyclobutane. Measured $(k_r/k_r^{A'}) = 0.90$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [2.19.4].	Rous..78F430
2.21	2-methylpropene $(CH_3)_2C{=}CH_2$	MeOH	6.25×10^4	1.6	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. E_a = 24 kJ mol^{-1}.	Koch 68F288
2.22	2-propenal $CH_2{=}CHCHO$	MeOH	1.6×10^3 $*1.1 \times 10^3$	89	-10	Od-15	S = MB. k derived using $k_d = 1.4 \times 10^5$ ($*1.0 \times 10^5$) s^{-1} [1.3].	Carm.73F479
2.23	1-cyclopropyl-2-methylpropene 	$(Me)_2CO$	$k_r = 8.6 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.66$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [2.19.4].	Rous..78F430
2.24	1,1-dicyclopropyl-propene 	$(Me)_2CO$	$k_r = 6.5 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.50$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [2.19.4].	Rous..78F430
2.25	1,1-dicyclopropyl-2-methylpropene 	$(Me)_2CO$	$k_r = 8.5 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.65$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [2.19.4].	Rous..78F430
		For more relative rates see		2.26.				
2.26	1,1-dicyclopropyl-2-methylpropene-d_6 	Me_2CO	$k_r = 8.5 \times 10^5$		rt	?	S = Eos, A' = 1,1-dicyclopropyl-2-methylpropene. Measured $(k_r/k_r^{A'}) = 1.0$. k_r derived using $k_r^{A'} = 8.5 \times 10^5$ dm^3 mol^{-1} s^{-1} [2.25]. $(k_r/k_r^{A'})$ measured as a product isotope effect.	Rous..78F430
2.27	(1-cyclopropylethylidene)cyclobutane 	$(Me)_2CO$	$k_r = 9.1 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.70$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [2.19.4].	Rous..78F430
2.28	2,3-dimethyl-1-butene $(CH_3)_2CHC(CH_3){=}CH_2$	MeOH	$k_r = 7.8 \times 10^3$		15	Ad-17 A'd	S = MB, A' = cyclohexene. Measured $(k_r/k_r^{A'}) = 1.7 \pm 0.4$. k_r derived using $k_r^{A'} = 4.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [2.54.1].	Kope.65F028

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.29	*cis*-2-butene $CH_3CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(5.5 \pm 2.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
2.30	*trans*-2-butene $CH_3CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(1.5 \pm 0.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
2.31	2-butene (*cis,trans* mix)	MeOH	8.0×10^3	12.5	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 42 kJ mol^{-1}.	Koch68F288
2.32	*trans*-2-butenal $CH_3CH=CHCHO$	MeOH	2.2×10^3 $*1.5 \times 10^3$	65	−10	Od-15	S = MB. k derived using $k_d = 1.4 \times 10^5$ ($*1.0 \times 10^5$) s^{-1} [*1.3.6*].	Carm.73F479
2.33	2-methyl-2-butene $CH_3CH=C(CH_3)_2$	MeOH(?)	1.8×10^6	5.5×10^{-2}	rt	?	Method not given. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
2.33.1		MeOH	1.7×10^5	6.0×10^{-1}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 6.7 kJ mol^{-1}.	Koch68F288
2.33.2		MeOH	1.8×10^6	5.5×10^{-2}	20	Od-15	S = tetrachloroeosin. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 6.3 kJ mol^{-1}.	Koch68F288
2.33.3		MeOH	1.7×10^6	6.0×10^{-2}	20	Od-15	S = tetrachloro-fluorescein. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 6.7 kJ mol^{-1}.	Koch68F288
2.33.4		MeOH	1.0×10^6	1.0×10^{-1}	20	Od-15	S = MB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 9.2 kJ mol^{-1}.	Koch68F288
2.33.5		MeOH	3.3×10^6	3.0×10^{-2}	20	Od-15	S = binaphthalene-thiophene. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 5.9 kJ mol^{-1}.	Koch68F288
2.33.6		MeOH	1.1×10^6	1.0×10^{-1}	?	?	Unpublished data. Method not given. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A357
2.33.7		$CHCl_3$	$(2.3 \pm 0.4) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
2.33.8		EtOH	4.8×10^4	1.65	rt	Ad-15	S = MB. k derived using $k_d = *7.9 \times 10^4$ s^{-1}. Reported values are suspect since r_{ox} depends on [O_2] and β value was determined from nonlinear data plots.	Brki..76F041
2.33.9		MeOH /*t*-BuOH (1:1) v:v	$k_r = 7.3 \times 10^5$		30	Pa-17 P'a	S = RB, A' = TME. Measured ($k_r^{A'}/k_r$) = 41. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

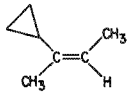
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.33.10		MeOH /*t*-BuOH (1:1) v:v	$k_r = 8.6 \times 10^5$		25	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = TME. Measured ($k_r^{A'}/k_r$) = 35. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.33.11		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.4 \times 10^6$		rt	Ad-17 A'd	S = RB, A' = TME. Measured ($k_r^{A'}/k_r$) = 22. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.33.12		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.0 \times 10^6$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/NaOCl, A' = TME. Measured ($k_r^{A'}/k_r$) = 15. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.33.13		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.3 \times 10^6$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A' = TME. Measured ($k_r^{A'}/k_r$) = 23. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
		For more relative rates see		2.40.27, 2.40.28, 2.42.3, 2.42.4, 2.43.1, 2.43.2, 2.52.7, 2.52.8, 2.56.14, 2.56.15, 3.12, 13.1, 13.2, 13.3, 13.4.				
2.34	*trans*-2-cyclopropyl-2-butene 	$(Me)_2CO$	$k_r = 6.9 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured ($k_r/k_r^{A'}$) = 0.53. k_r derived using $k_r^{A'}$ = 1.3 × 10^6 dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430
2.35	2,3-dimethyl-2-butene (TME) $(CH_3)_2C{=}C(CH_3)_2$	MeOH(?)	3.3 × 10^7	3.0 × 10^{-3}	rt	?	Method not given. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Goll62F005
2.35.1		MeOH	1.6 × 10^7	6.2 × 10^{-3}	20	Od-15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 2.1 kJ mol^{-1}.	Koch68F288
2.35.2		MeOH	2.2 × 10^7	(4.6 ± 0.5) × 10^{-3}	23	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn..71F398
2.35.3		MeOH	(4.0 ± 1.0) × 10^7		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Merk.71M325
2.35.4		$CHCl_3$	(5.8 ± 0.9) × 10^7		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67 × 10^4 s^{-1} [*1.5*].	Monr78A005
2.35.5		EtOH	1.6 × 10^7 *3.2 × 10^7		rt	Od-23	S = RB, A' = hexamethylenedithiocarbamate. Measured $k/(k_d + k_A[A']) =$ 270 at [A'] = 2.8 × 10^{-4} mol dm^{-3}. k derived using $k_{A'}$ = 1.5 × 10^8 dm^3 mol^{-1} s^{-1} [*11.42*] and k_d = 1.0 × 10^4 (*7.9 × 10^4) s^{-1} [*1.10.3*].	Yama..72F116

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.35.6	EtOH	1.4×10^5	5.6×10^{-1}	rt	Ad–15	S = MB. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*]. Reported values are suspect since r_{ox} depends on [O_2] and β value was determined from nonlinear data plots.	Brki...76F041
2.35.7	$(Me)_2CO$	5.4×10^7 *4.3×10^7	$(7.2 \pm 0.2) \times 10^{-4}$	15	A′d–16	S = RB, A′ = DPBF. k derived using k_d = 3.8×10^4 (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.35.8	*n*–BuOH	1.2×10^7	$(4.4 \pm 0.5) \times 10^{-3}$	23	A′d–16	S = MB, A′ = DPBF. k derived using k_d = 5.2×10^4 s^{-1} [*1.24*].	Youn..71F398
2.35.9	*t*–BuOH	1.0×10^7	$(2.9 \pm 0.3) \times 10^{-3}$	23	A′d–16	S = MB, A′ = DPBF. k derived using k_d = 3.0×10^4 s^{-1} [*1.25*].	Youn..71F398
2.35.10	C_5H_5N	1.6×10^7		~10	A′d–20	S = A′ = DPBF. Measured ($k/k_{A'}$) = 2.6×10^{-2}. k derived using $k_{A'}$ = *6.3×10^8 dm^3 mol^{-1} s^{-1} [*A3.17*].	Wils66F014
2.35.11	C_5H_5N	4.5×10^7	1.3×10^{-3}	12	Pa–20	S = thionine,MB,DMA A′ = DMA. k derived using k_d = 5.9×10^4 s^{-1} [*1.29.1*]. β is the same for all 3 S.	Kram.73F202
2.35.12	C_6H_6	5.2×10^7	7.7×10^{-4}	25	A′d–23	S = A′ = DMA. k derived using $\beta_{A'}$ = 3.0×10^{-4} mol dm^{-3} [*3.53.21*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.35.13	C_6H_6	3.3×10^7	1.2×10^{-3}	25	A′d–23	S = A′ = DMBA. k derived using $\beta_{A'}$ = 7.1×10^{-4} mol dm^{-3} [*3.61.2*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.35.14	C_6H_6	3.2×10^7	1.25×10^{-3}	25	A′d–23	S = A′ = Tetr. k derived using $\beta_{A'}$ = 1.7×10^{-3} mol dm^{-3} [*3.62.4*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.35.15	C_6H_6	5.6×10^7	7.14×10^{-4}	25	A′d–23	S = A′ = Rub. k derived using $\beta_{A'}$ = 3.0×10^{-4} mol dm^{-3} [*3.63.15*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.35.16	$C_6H_5CH_3$	4.2×10^7		rt	A′d–5	S = Naph, A′ = DPBF. Sensitizer excited with pulsed electron beam (10 MeV).	Gorm..78E263
2.35.17	MeOH /*t*–BuOH (1:1) v:v	3.4×10^7 (est)	$(2.3 \pm 0.3) \times 10^{-3}$	rt	A′d–16	S = RB, A′ = DPBF. k estimated using k_d = 7.9×10^4 s^{-1} (calc).	Youn..71F398
	For more relative rates see		2.3.2, 2.12.3, 2.33.9–13, 2.42.1–2, 2.58.1, 2.86.2–4, 2.91.5–6, 3.35, 3.35.1, 3.43, 3.43.1, 3.53.15, 3.53.26, 3.56.5, 3.63.10–11, 4.16, 4.16.1, 5.29.15–17, 5.36.89, 6.21, 6.21.1–8, 7.1, 7.1.1, 11.31.4, 14.32.6.				

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

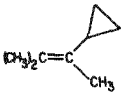
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.36	2-cyclopropyl-3-methyl-2-butene 	$(Me)_2CO$	$k_r = 9.9 \times 10^5$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.76$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430
2.37	1-pentene $CH_3(CH_2)_2CH=CH_2$	CCl_4/MeOH (96:4) v:v	$(1.0 \pm 0.4) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
2.38	*cis*-2-pentene $CH_3CH_2CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(4.0 \pm 1.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
2.39	*trans*-2-pentene $CH_3CH_2CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(2.0 \pm 0.8) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
2.40	2-methyl-2-pentene (2M2P) $CH_3CH_2CH=C(CH_3)_2$	MeOH(?)	5.6×10^5	1.8×10^{-1}	rt	?	Method not given. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
2.40.1		MeOH	7.7×10^5	1.3×10^{-1}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. $E_a =$ 8.4 kJ mol^{-1}.	Koch68F288
2.40.2		MeOH	6.25×10^5	$(1.6 \pm 0.3) \times 10^{-1}$	25	Pa-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Foot.71F356
2.40.3		MeOH	7.7×10^5	$(1.3 \pm 0.1) \times 10^{-1}$	25	Pa-15	S = chlorophyll-b. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Foot.71F356
2.40.4		MeOH	5.0×10^5	$(2.0 \pm 0.8) \times 10^{-1}$	25	Pa-15	S = chlorophyll-a. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Foot.71F356
2.40.5		MeOH	6.7×10^5	$(1.5 \pm 0.2) \times 10^{-1}$	25	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn..71F398
2.40.6		MeOH	5.3×10^5	$(1.9 \pm 0.4) \times 10^{-1}$	rt	Pa-15	S = ZnTPP. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Foot.71F580
2.40.7		MeOH	6.25×10^5	1.6×10^{-1}	-20	Od-14 27	S = RB, A' = α-terpinene. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Chai.76F909
2.40.8		$CHCl_3$	$(1.9 \pm 0.3) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
2.40.9		CS_2	6.25×10^4	$(8.0 \pm 1.0) \times 10^{-2}$	0	Pa-15	S = ZnTPP. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Foot.71F356
2.40.10		CH_3CN	1.8×10^6	1.4×10^{-2}	rt	Pa-15	S = RB. k derived using $k_d = *2.55 \times 10^4$ s^{-1} [*1.17.2*].	Foot.71F580
2.40.11		CH_3CN	1.4×10^6	1.8×10^{-2}	rt	Od-15	S = RB. k derived using $k_d = *2.55 \times 10^4$ s^{-1} [*1.17.2*].	Smit..75F166
2.40.12		C_2H_5I	2.3×10^6 (est)	$(1.1 \pm 0.3) \times 10^{-1}$	25	Pa-15	S = ZnTPP. k estimated using $k_d = 2.5 \times 10^5$ s^{-1} [*1(a).0*].	Foot.71F356

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.40.13		$(Me)_2SO$	7.4×10^5 (est)	$(7.0 \pm 1.0) \times 10^{-2}$	25	Pa-15	S = RB. k estimated using $k_d = 5.2 \times 10^4$ s^{-1} [*1(a).1*].	Foot.71F356
2.40.14		$(Me)_2SO$	9.5×10^5 (est)	$(5.5 \pm 0.1) \times 10^{-2}$	rt	A'd-16	S = RB, A' = DPBF. k estimated using $k_d = 5.2 \times 10^4$ s^{-1} [*1(a).1*].	Guir.76E072
2.40.15		methyl acetate	5.3×10^5 (est)	$(4.0 \pm 2.0) \times 10^{-2}$	25	Pa-15	S = RB. k estimated using k_d(ethyl acetate) = 2.1×10^4 s^{-1} [*1.28*].	Foot.71F356
2.40.16		$(Me)_2CO$	3.9×10^5	$(8.0 \pm 1.0) \times 10^{-2}$	25	Pa-15	S = RB. k derived using k_d = *3.1×10^4 s^{-1} [*1.22.2*].	Foot.71F356
2.40.17		t-BuOH	3.7×10^5	$(8.1 \pm 0.8) \times 10^{-2}$	25	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Youn..71F398
2.40.18		C_5H_5N	1.2×10^6	$(5.0 \pm 1.0) \times 10^{-2}$	25	Pa-15	S = RB. k derived using k_d = 5.9×10^4 s^{-1} [*1.29.1*].	Foot.71F356
2.40.19		C_5H_5N	1.4×10^6	4.3×10^{-2}	rt	Od-15	S = RB. k derived using k_d = 5.9×10^4 s^{-1} [*1.29.1*].	Smit..75F166
2.40.20		$C_6H_{11}OH$	9.0×10^5	$(7.0 \pm 1.0) \times 10^{-2}$	25	Pa-15	S = RB. k derived using k_d = 6.3×10^4 s^{-1} [*1.31*].	Foot.71F356
2.40.21		C_6H_6	1.7×10^5	$(2.3 \pm 1.2) \times 10^{-1}$	rt	Pa-15	S = ZnTPP. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Foot.71F580
2.40.22		C_6H_6	4.0×10^5	$(1.0 \pm 0.1) \times 10^{-1}$	25	Pa-15	S = ZnTPP. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Foot.71F356
2.40.23		C_6H_6	7.5×10^5	5.3×10^{-2}	rt	Od-15	S = azine. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Smit..75F166
2.40.24		C_6H_5Br	2.6×10^5	$(5.0 \pm 3.0) \times 10^{-2}$	25	Pa-15	S = ZnTPP. k derived using k_d = 1.3×10^4 s^{-1} [*1.34*].	Foot.71F356
2.40.25		methoxy-benzene	3.1×10^5 (est)	$(1.3 \pm 0.2) \times 10^{-1}$	25	Pa-15	S = ZnTPP. k estimated using $k_d(C_6H_5CH_3)$ = 4.0×10^4 s^{-1} [*1.36*].	Foot.71F356
2.40.26		1,3-di-methoxy-benzene	2.7×10^5 (est)	$(1.5 \pm 0.4) \times 10^{-1}$	25	Pa-15	S = ZnTPP. k estimated using $k_d(C_6H_5CH_3)$ = 4.0×10^4 s^{-1} [*1.36*].	Foot.71F356
2.40.27		MeOH /t-BuOH (1:1) v:v	$k_r = 1.1 \times 10^6$		30	Pa-17 P'a	S = RB, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.32. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.40.28		MeOH /t-BuOH (1:1) v:v	$k_r = 1.2 \times 10^6$		25	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.28. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.40.29		MeOH /t-BuOH (1:1) v:v	6.6×10^5 (est)	$(1.2 \pm 0.2) \times 10^{-1}$	rt	A'd-16	S = RB, A' = DPBF. k estimated using k_d = 7.9×10^4 s^{-1} (calc).	Youn..71F398

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.40.30		C_6H_6/MeOH (4:1) v:v	7.6×10^5	$(5.0 \pm 0.5) \times 10^{-2}$	rt	Pa–15	S = MB. k derived using k_d = 3.8×10^4 s^{-1} [*1.49*].	Foot.71F356
		For more relative rates see		2.45, 2.45.1, 2.46, 2.46.1, 2.56.12–13, 2.119, 2.121, 2.123, 2.126, 2.126.1, 2.130.9, 2.132, 4.7.2, 4.7.8–9, 4.9.1, 4.12.4.				
2.41	2-methyl-2-pentene-4-ol $CH_3CH(OH)CH=C(CH_3)_2$	MeOH	1.2×10^4	8.4	–20	Od–14 27	S = RB, A′ = α-terpinene. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Chai.76F909
2.42	*cis*-3-methyl-2-pentene $CH_3CH_2C(CH_3)=CHCH_3$	$CHCl_3$	$(2.0 \pm 0.3) \times 10^6$		rt	A′d–33	S = A′ = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
2.42.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 8.3 \times 10^5$		rt	Ad–17 A′d	S = RB, A′ = TME. Measured ($k_r^{A'}/k_r$) = 36. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.42.2		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.2 \times 10^6$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/NaOCl, A′ = TME. Measured ($k_r^{A'}/k_r$) = 25. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.42.3		MeOH /*t*-BuOH (1:1) v:v	$k_r = 8.3 \times 10^5$		rt	Ad–17 A′d	S = RB, A′ = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.8. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.42.4		MeOH /*t*-BuOH (1:1) v:v	$k_r = 6.0 \times 10^5$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A′ = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 2.5. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.42.5		EtOH /*i*-PrOH (1:1) v:v	1.3×10^6 (est)	5.0×10^{-2}	19	Od–14 27	S = RB, A′ = DMF. k estimated using $k_d = 6.7 \times 10^4$ s^{-1} (calc).	Schu..78F464
2.43	*trans*-3-methyl-2-pentene $CH_3CH_2C(CH_3)=CHCH_3$	$CHCl_3$	$(1.5 \pm 0.3) \times 10^6$		rt	A′d–33	S = A′ = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
2.43.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.2 \times 10^6$		rt	Ad–17 A′d	S = RB, A′ = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.2. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.43.2		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.1 \times 10^6$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A′ = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.4. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.43.3		MeOH /*t*-BuOH (1:1) v:v	$k_r = 4.4 \times 10^6$		rt	Ad-17 A'd	S = RB, A' = 1-methylcyclohexene. Measured ($k_r/k_r^{A'}$) = 22. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Higg..68F292
2.43.4		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.4 \times 10^6$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/Ca(OCl)$_2$, A' = 1-methylcyclohexene. Measured ($k_r/k_r^{A'}$) = 7. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Higg..68F292
2.43.5		EtOH /*i*-PrOH (1:1) v:v	1.1 × 10^6 (est)	6.0 × 10^{-2}	19	Od-14 27	S = RB, A' = DMF. k estimated using k_d = 6.7 × 10^4 s^{-1} (calc).	Schu..78F464
2.44	3-methyl-2-pentene (*cis,trans* mix)	C_6H_5Cl	1.0 × 10^6 (est)	1.6 × 10^{-2}	25	Ad-15	S = TPP. k estimated using k_d = 1.6 × 10^4 s^{-1} [*1(a).5*].	Carl..74F341
2.45	*cis*-4-methyl-2-pentene $(CH_3)_2CHCH{=}CHCH_3$	MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.1 \times 10^4$		30	Pa-17 P'a	S = RB, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 1.4 × 10^{-2}. k_r derived using $k_r^{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.45.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 8.9 \times 10^3$		3-4	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 1.1 × 10^{-2}. k_r derived using $k_r^{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.45.2		MeOH /*t*-BuOH (1:1) v:v	9.9 × 10^3 (est)	8.0 ± 0.8	rt	A'd-16	S = RB, A' = DPBF. k estimated using k_d = 7.9 × 10^4 s^{-1} (calc).	Youn..71F398
		For more relative rates see		2.54.2.				
2.46	*trans*-4-methyl-2-pentene $(CH_3)_2CHCH{=}CHCH_3$	MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.0 \times 10^3$		30	Pa-17 P'a	S = RB, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 2.5 × 10^{-3}. k_r derived using $k_r^{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.46.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.6 \times 10^3$		3-4	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 2.0 × 10^{-3}. k_r derived using $k_r^{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.47	2,4-dimethyl-2-pentene $(CH_3)_2CHCH{=}C(CH_3)_2$	MeOH(?)	7.7 × 10^4	1.3	rt	?	Method not given. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Goll62F005
2.47.1		$CHCl_3$	(4.3 ± 0.7) × 10^5		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67 × 10^4 s^{-1} [*1.5*].	Monr78A005
2.48	2,3,4-trimethyl-2-pentene $(CH_3)_2CHC(CH_3){=}C(CH_3)_2$	$CHCl_3$	(3.9 ± 0.6) × 10^7		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67 × 10^4 s^{-1} [*1.5*].	Monr78A005

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.49	2,4,4-trimethyl-2-pentene $(CH_3)_3CCH{=}CH(CH_3)_2$	MeOH(?)	2.4×10^4	4.2	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.50	cyclopentene 	MeOH	$k_r = 7.0 \times 10^4$		15	Ad-17 A'd	S = MB, A' = 2,3-dimethylcyclohexene. Measured ($k_r^{A'}/k_r$) = 3.0 ± 0.1. k_r derived using $k_r^{A'}$ = *2.1×10^5 dm^3 mol^{-1} s^{-1} [*2.59*].	Kope.65F028
2.51	3,5-dioxacyclopentene 	*For more relative rates see* (Me)$_2$CO	1.2×10^7 *9.5×10^6	2.53. $(3.28 \pm .04) \times 10^{-3}$	15	A'd-16	S = RB, A' = DPBF. k derived using k_d = 3.8×10^4 (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
2.52	1-methylcyclopentene 	MeOH	$k_r = 2.1 \times 10^5$		15	Ad-17 A'd	S = MB, A' = 1,2-dimethylcyclohexene. Measured ($k_r^{A'}/k_r$) = 7.5 ± 0.7. k_r derived using $k_r^{A'}$ = 1.6×10^7 dm^3 mol^{-1} s^{-1} [*2.58.1*].	Kope.65F028
2.52.1		$CHCl_3$	$(2.7 \pm 0.4) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
2.52.2		CH_3CN	$k_r = 1.5 \times 10^6$		rt	?	S = MB, A' = 1-methylcyclohexene. Measured ($k_r/k_r^{A'}$) = 7.7. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.52.3		C_6H_6	2.3×10^6	1.75×10^{-2}	25	A'd-23	S = A' = DMA. k derived using $\beta_{A'}$ = 3.0×10^{-4} mol dm^{-3} [*3.53.21*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.52.4		C_6H_6	2.5×10^6	1.6×10^{-2}	25	A'd-23	S = A' = DMBA. k derived using $\beta_{A'}$ = 7.1×10^{-4} mol dm^{-3} [*3.61.2*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.52.5		C_6H_6	2.3×10^6	1.75×10^{-2}	25	A'd-23	S = A' = Tetr. k derived using $\beta_{A'}$ = 1.7×10^{-3} mol dm^{-3} [*3.62.4*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga70E079
2.52.6		C_6H_6	2.2×10^6	1.8×10^{-2}	25	A'd-23	S = A' = Rub. k derived using $\beta_{A'}$ = 3.0×10^{-4} mol dm^{-3} [*3.63.15*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.52.7		MeOH /t-BuOH (1:1) v:v	$k_r = 1.5 \times 10^6$		rt	Ad-17 A'd	S = RB, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.0. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.52.8		MeOH /t-BuOH (1:1) v:v	$k_r = 9.4 \times 10^5$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 1.6. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.52.9		?	$k_r = 1.2 \times 10^6$		rt	?	Experimental method unclear, A' = 1-methylcyclohexene. Measured ($k_r/k_r^{A'}$) = 6.2. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Foot.71F580
		For more relative rates see		2.56.1-5.				
2.53	2-hexene $CH_3(CH_2)_2CH{=}CHCH_3$	MeOH	$k_r = 3.9 \times 10^4$		15	Ad-17 A'd	S = MB, A' = cyclopentene. Measured ($k_r^{A'}/k_r$) = 1.8 ± 0.4. k_r derived using $k_r^{A'} = 7.0 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.50*].	Kope.65F028
		For more relative rates see		2.54.1.				
2.54	cyclohexene 	MeOH(?)	3.8×10^3	26	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.54.1		MeOH	$k_r = 4.6 \times 10^3$		15	Ad-17 A'd	S = MB, A' = 2-hexene. Measured ($k_r^{A'}/k_r$) = 8.5 ± 0.2. k_r derived using $k_r^{A'} = 3.9 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.53*].	Kope.65F028
2.54.2		MeOH /t-BuOH (1:1) v:v	$k_r = 2.0 \times 10^3$		30	Pa-17 P'a	S = RB, A' = *cis*-4-methyl-2-pentene. Measured ($k_r^{A'}/k_r$) = 5.4. k_r derived using $k_r^{A'}$ = 1.1×10^4 dm^3 mol^{-1} s^{-1} [*2.45*].	Higg..68F292
2.54.3		C_6H_6/MeOH (3:1) v:v	2.0×10^4	3.1	25	Ad-15	S = MB. k derived using $k_d = 6.25 \times 10^4$ s^{-1}.	Kret.78F586
		For more relative rates see		2.28, 2.57, 2.85.				
2.55	3,6-dioxacyclohexene 	$(Me)_2CO$	3.6×10^5 *1.4×10^5		8	?	S = ?, A' = Car. Measured ($k/k_{A'}$) = 1.2×10^{-5}. k derived using $k_{A'} = 3 \times 10^{10}$ (*1.2×10^{10}) dm^3 mol^{-1} s^{-1}.	Bart..70F733
2.55.1		$(Me)_2CO$	2.2×10^5 *1.8×10^5	(1.76 ± .02) $\times 10^{-1}$	15	A'd-16	S = RB, A' = DPBF. k derived using k_d = 3.8×10^4 (*3.1×10^4) s^{-1} [*1.22*].	Fale77F876
		For more relative rates see		2.1, 2.1.2, 2.2.1, 2.3-4, 2.56.7, 2.63, 3.24, 15.12.				

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.56	1-methylcyclo-hexene 	MeOH(?)	8.3×10^4	1.2	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.56.1		MeOH	$k_r = 2.0 \times 10^5$		15	Ad-17 A'd	S = MB, A' = 1-methyl-cyclopentene. Measured ($k_r^{A'}/k_r$) = 8.6 ± 0.9. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Kope.65F028
2.56.2		MeOH	$k_r = 1.6 \times 10^5$		15	Ad-17 A'd	S = RB, A' = 1-methyl-cyclopentene. Measured ($k_r^{A'}/k_r$) = 11.5 ± 1.9. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Kope.65F028
2.56.3		MeOH	$k_r = 1.7 \times 10^5$		15	Ad-17 A'd	S = Eos, A' = 1-methylcyclopentene. Measured ($k_r^{A'}/k_r$) = 10.8 ± 1.4. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Kope.65F028
2.56.4		MeOH	$k_r = 2.0 \times 10^5$		15	Ad-17 A'd	S = erythrosin-B, A'= 1-methylcyclopentene. Measured ($k_r^{A'}/k_r$) = 8.8 ± 1.6. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Kope.65F028
2.56.5		MeOH	$k_r = 1.9 \times 10^5$		15	Ad-17 A'd	S = hematoporphyrin, A' = 1-methylcyclopentene. Measured ($k_r^{A'}/k_r$) = 9.4 ± 1.8. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Kope.65F028
2.56.6		$CHCl_3$	$(3.6 \pm 0.6) \times 10^5$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
2.56.7		$(Me)_2CO$	$k_r = 2.1 \times 10^5$ *1.7×10^5		8	?	S = ?, A' = p-dioxene. Measured ($k_r/k_r^{A'}$) = 9.6×10^{-1}. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
2.56.8		C_6H_6	3.0×10^5	1.3×10^{-1}	25	A'd-23	S = A' = DMA. k derived using $\beta_{A'}$ = 3.0×10^{-4} mol dm^{-3} [*3.53.21*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.56.9		C_6H_6	3.3×10^5	1.2×10^{-1}	25	A'd-23	S = A' = DMBA. k derived using $\beta_{A'}$ = 7.1×10^{-4} mol dm^{-3} [*3.61.2*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

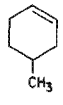
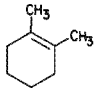
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.56.10		C_6H_6	2.9×10^5	1.4×10^{-1}	25	A'd-23	S = A' = Tetr. k derived using $\beta_{A'} = 1.7 \times 10^{-3}$ mol dm^{-3} [*3.62.4*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.56.11		C_6H_6	2.7×10^5	1.47×10^{-1}	25	A'd-23	S = A' = Rub. k derived using $\beta_{A'} = 3.0 \times 10^{-4}$ mol dm^{-3} [*3.63.15*] and k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
2.56.12		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.8 \times 10^5$		30	Pa-17 P'a	S = RB, A' = 2M2P. Measured ($k_r^{A'}/k_r$) = 4.5. k_r derived using $k_r^{A'}$ = *8.1×10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.56.13		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.1 \times 10^5$		3-4	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = 2M2P. Measured ($k_r^{A'}/k_r$) = 3.9. k_r derived using $k_r^{A'}$ = *8.1×10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Higg..68F292
2.56.14		MeOH /*t*-BuOH (1:1) v:v	$k_r = 6.5 \times 10^4$		rt	Ad-17 A'd	S = RB, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 23. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
2.56.15		MeOH /*t*-BuOH (1:1) v:v	$k_r = 7.5 \times 10^4$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A' = 2-methyl-2-butene. Measured ($k_r^{A'}/k_r$) = 20. k_r derived using $k_r^{A'}$ = *1.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.1*].	Higg..68F292
		For more relative rates see		2.5, 2.7, 2.43.3-4, 2.52.2, 2.52.9, 2.59, 2.64, 2.71, 2.74.6, 2.75.1, 2.77, 2.84, 2.90.1-6.				
2.57	4-methylcyclohexene 	MeOH	$k_r = 3.1 \times 10^3$		15	Ad-17 A'd	S = MB, A' = cyclohexene. Measured ($k_r^{A'}/k_r$) = 1.5 ± 0.2. k_r derived using $k_r^{A'} = 4.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.54.1*].	Kope.65F028
2.58	1,2-dimethylcyclohexene 	MeOH(?)	3.3×10^6	3.0×10^{-2}	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.58.1		MeOH	$k_r = 1.6 \times 10^7$		15	Ad-17 A'd	S = MB, A' = TME. Measured ($k_r^{A'}/k_r$) = 1.9 ± 0.2. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Kope.65F028
2.58.2		MeOH	$(1.0 \pm 0.25) \times 10^7$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Merk.72F260
2.58.3		$CHCl_3$	$(3.0 \pm 0.5) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
		For more relative rates see		2.52.				

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

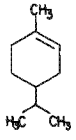
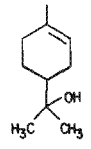
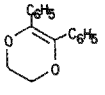
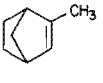
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.59	2,3-dimethyl-cyclohexene 	MeOH	k_r = *2.1 × 10^5		15	Ad-17 A'd	S = MB, A' = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 1.07 ± 0.03. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Kope.65F028
		For more relative rates see		2.50.				
2.60	carvomenthene 	MeOH	≈ 1.0 × 10^5	≈ 1.0	20	Od-15	S = MB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 13 kJ mol^{-1}.	Koch68F288
2.61	terpinolene 	MeOH	≈ 2.0 × 10^6	≈ 5.0 × 10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 1.7 kJ mol^{-1}.	Koch68F288
2.62	3,6-endoperoxy-cyclohexene 	MeOH	6.7 × 10^2	150	20	Od-15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 26 kJ mol^{-1}.	Koch68F288
2.63	1,2-diphenyl-3,6-dioxacyclohexene 	$(Me)_2CO$	k_r = 1.3 × 10^7 *1.0 × 10^7		8	?	S = ?, A' = *p*-dioxene. Measured ($k_r/k_r^{A'}$) = 58. k_r derived using $k_r^{A'}$ = 2.2 × 10^5 (*1.8 × 10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
2.64	2-methylnorborn-2-ene 	CH_3CN	k_r = 2.8 × 10^4		rt	?	S = MB, A' = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 0.14. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.64.1		CH_3CN	k_r = 4.0 × 10^4		rt	Ad-17 A'd	S = MB, A' = 2-methyl-idenenorbornane. Measured ($k_r/k_r^{A'}$) = 3.1. k_r derived using $k_r^{A'}$ = 1.3 × 10^4 dm^3 mol^{-1} s^{-1} [*2.71*].	Jeff.74F647
2.64.2		CH_3CN	k_r = 4.9 × 10^4		0	Ad-17 A'd	S = MB, A' = 2-methyl-idenenorborn-5-ene. Measured ($k_r/k_r^{A'}$) = 13.5. k_r derived using $k_r^{A'}$ = 3.6 × 10^3 dm^3 mol^{-1} s^{-1} [*2.94b*].	Jeff..78F149

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

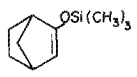
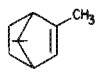
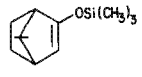
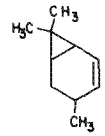
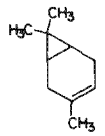
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.65	2-(trimethyl-siloxy)norborn-2-ene 	$CDCl_3$	$(k_r/k_r^{A'}) = 8.4$		rt	Ad-17 A'd	S = *meso*-TPP, A' = 7,7-dimethyl-2-(trimethyl-siloxy)norborn-2-ene.	Jeff.78F290
		For more relative rates see		2.67.				
2.66	2,7,7-trimethyl-norborn-2-ene 	MeOH(?)	1.2×10^4	8.2	?	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll68F289
2.66.1		CH_3CN	$k_r = 1.0 \times 10^3$		rt	Ad-17 A'd	S = MB, A' = 2-methyl-idenenorbornane. Measured $(k_r/k_r^{A'}) = 7.7 \times 10^{-2}$. k_r derived using $k_r^{A'} = 1.3 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.71*].	Jeff.74F647
2.66.2		CH_3CN	$k_r = 1.2 \times 10^3$		0	Ad-17 A'd	S = MB, A' = 2-methyl-norborn-2-ene. Measured $(k_r^{A'}/k_r) = 40.0$. k_r derived using $k_r^{A'} = 4.9 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.64.2*].	Jeff..78F149
2.67	7,7-dimethyl-2-(trimethylsiloxy)-norborn-2-ene 	$CDCl_3$	$(k_r/k_r^{A'}) = 0.12$		rt	Ad-17 A'd	S = *meso*-TPP, A' = 2-(trimethyl-siloxy)norborn-2-ene.	Jeff.78F290
		For more relative rates see		2.65, 2.95, 2.96.				
2.68	Δ^2-carene 	MeOH(?)	5.9×10^5	1.7×10^{-1}	rt	?	Method not reported. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll68F289
2.69	Δ^3-carene 	MeOH(?)	2.5×10^5	4.0×10^{-1}	rt	?	Method not reported. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll68F289

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

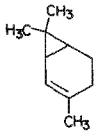
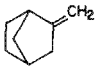
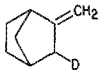
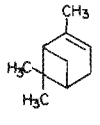
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.70	Δ^4–carene 	MeOH(?)	4.8×10^5	2.1×10^{-1}	rt	?	Method not reported. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll68F289
2.71	2-methylidene-norbornane 	CH_3CN	$k_r = 1.3 \times 10^4$		rt	?	S = MB, A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 0.65. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.71.1		CH_3CN	$k_r = 1.5 \times 10^4$		0	Ad-17 A′d	S = MB, A′ = 2-methyl-idenenorborn-5-ene. Measured ($k_r/k_r^{A'}$) = 4.3. k_r derived using $k_r^{A'} = 3.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.94b*].	Jeff..78F149
2.71.2		CH_3CN	$k_r = 1.6 \times 10^4$		0	Ad-17 A′d	S = MB, A′ = 2,7,7-tri-methylnorborn-2-ene. Measured ($k_r/k_r^{A'}$) = 13.0. k_r derived using $k_r^{A'} = 1.2 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.66.2*].	Jeff..78F149
		For more relative rates see		2.64.1, 2.72, 2.73, 2.74.7, 2.75.2.				
2.72	*exo*-2-methylidene-norbornane-3-*d* 	CH_3CN	$k_r = 1.5 \times 10^4$		rt	Ad-17 A′d	S = MB, A′ = 2-methyl-idenenorbornane. Measured ($k_r/k_r^{A'}$) = 1.14 ± 0.01. k_r derived using $k_r^{A'} = 1.3 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.71*].	Jeff.74F647
2.73	*endo*-2-methylidene-norbornane-3-*d*	CH_3CN	$k_r = 1.3 \times 10^4$		rt	Ad-17 A′d	S = MB, A′ = 2-methyl-idenenorbornane. Measured ($k_r/k_r^{A'}$) = 1.02 ± 0.01. k_r derived using $k_r^{A'} = 1.3 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.71*].	Jeff.74F647
2.74	α-pinene 	MeOH(?)	1.2×10^4	8.2	rt	?	Method not reported. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll68F289
2.74.1		MeOH	2.0×10^4	5.0	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 19 kJ mol^{-1}.	Koch68F288
2.74.2		MeOH	2.6×10^4	3.8	20	Od-15	S = tetrachloroeosin. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 17 kJ mol^{-1}.	Koch68F288
2.74.3		MeOH	2.0×10^5	5.0×10^{-1}	20	Od-15	S = tetrachloro-fluorescein. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 17 kJ mol^{-1}.	Koch68F288

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

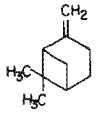
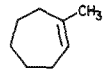
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.74.4		MeOH	1.4×10^4	7.0	20	Od-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 20 kJ mol^{-1}.	Koch68F288
2.74.5		MeOH	3.6×10^4	2.8	20	Od-15	S = binaphthalene-thiophene. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 21 kJ mol^{-1}.	Koch68F288
2.74.6		CH_3CN	$k_r = 5.0 \times 10^4$		rt	?	S = MB, A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 0.25. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.75	β-pinene 	MeOH	$\approx 1.0 \times 10^5$	≈ 1.0	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 21 kJ mol^{-1}.	Koch68F288
2.75.1		CH_3CN	$k_r = 3.8 \times 10^4$		rt	Ad-17 A′d	S = MB, A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 0.19. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Jeff....73F664
2.75a	7,7-dimethyl-2-methylidene-norbornane 	CH_3CN	$k_r = 3.4 \times 10^3$		rt	Ad-17 A′d	S = MB, A′ = 2-methyl-idenenorbornane. Measured ($k_r/k_r^{A'}$) = 2.6×10^{-1}. k_r derived using $k_r^{A'} = 1.3 \times 10^4$ dm^3 mol^{-1} s^{-1} [*2.71*].	Jeff.74F647
2.75a.1		CH_3CN	$k_r = 4.1 \times 10^3$		0	Ad-17 A′d	S = MB, A′ = 2,7,7-*tri*-methylnorborn-2-ene. Measured ($k_r/k_r^{A'}$) = 3.4. k_r derived using $k_r^{A'} = 1.2 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.66.2*].	Jeff..78F149
2.76	1-heptene $CH_3(CH_2)_4CH=CH_2$	CCl_4/MeOH (96:4) v:v	$(1.5 \pm 0.5) \times 10^3$		rt	A′d-8	S = MB, A′ = DPBF, ruby laser (694 nm).	Bort...77F162
2.77	1-methylcyclo-heptene 	?	$k_r = 1.9 \times 10^6$		rt	?	Experimental method unclear, A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 9.4. k_r derived using $k_r^{A'}$ = *2.0×10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Foot.71F580
2.78	*trans*-4-methyl-4-octene $CH_3(CH_2)_2CH=C(CH_3)(CH_2)_2CH_3$	MeOH	5.0×10^5	2.0×10^{-1}	-20	Od-14 27	S =RB, A′ = α-terpinene. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Chai.76F909
2.79	*cis*-4-methyl-4-octene $CH_3(CH_2)_2CH=C(CH_3)(CH_2)_2CH_3$	MeOH	3.3×10^5	3.4×10^{-1}	-20	Od-14 27	S =RB, A′ = α-terpinene. k derived using k_d = 1.1×10^5 s^{-1} [1.3.4].	Tani.79F074

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

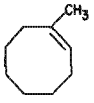
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.80	4-methyl-4-octene (46% *trans*,54% *cis*)	MeOH	3.7×10^5	2.7×10^{-1}	-20	Od-14 27	S =RB, A′ = α-terpinene. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Chai.76F909
2.81	4-methyl-4-octene (25% *trans*, 75% *cis*)	MeOH	3.4×10^5	2.9×10^{-1}	-20	Od-14 27	S =RB, A′ = α-terpinene. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Chai.76F909
2.82	3,7-dimethyl-6-octen-1-ol $(CH_3)_2C{=}CHCH_2CH_2CH(CH_3)CH_2CH_2OH$	MeOH	6.25×10^5	1.6×10^{-1}	20	Pa-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
2.82.1		MeOH	6.25×10^5	1.6×10^{-1}	20	Pa-15	S = Ery. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
2.82.2		MeOH	6.7×10^5	1.5×10^{-1}	20	Pa-15	S = Eos. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
2.82.3		*n*-BuOH	4.7×10^5	1.1×10^{-1}	20	Pa-15	S = RB. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Goll62F005
2.82.4		*n*-BuOH	4.3×10^5	1.2×10^{-1}	20	Pa-15	S = Eos. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Goll62F005
2.82.5		MeOH/H_2O (7:3) v:v	3.5×10^6 (est)	6.0×10^{-2}	20	Pa-15	S = RB. k estimated using $k_d = 2.1 \times 10^5$ s^{-1} (calc).	Goll62F005
2.82.6		MeOH/H_2O (7:3) v:v	3.5×10^6 (est)	6.0×10^{-2}	20	Pa-15	S = Eos. k estimated using $k_d = 2.1 \times 10^5$ s^{-1} (calc).	Goll62F005
2.83	cyclooctene 	EtOH	$(k_r/k_r^{A'}) = 1.43 \times 10^{-1}$		rt	Ad-17 A′d	S = MB, A′ = 1,5-cyclooctadiene.	Mats...71F581
2.84	1-methylcyclo-octene 	?	$k_r = 3.0 \times 10^5$		rt	?	Experimental method unclear, A′ = 1-methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 1.5$. k_r derived using $k_r^{A'} = *2.0 \times 10^5$ dm^3 mol^{-1} s^{-1} [*A3.5*].	Foot.71F580
2.85	1-nonene $CH_3(CH_2)_6CH{=}CH_2$	MeOH	$k_r = 4.6 \times 10^2$		15	Ad-17 A′d	S =MB, A′ = cyclohexene. Measured $(k_r^{A'}/k_r) = 10$. k_r derived using $k_r^{A'} = 4.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.54.1*].	Kope.65F028
2.86	cyclopentadiene 	MeOH	2.3×10^7	4.4×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. $E_a = 1.3$ kJ mol^{-1}.	Koch68F288
2.86.1		MeOH	2.4×10^7	4.1×10^{-3}	20	Od-15	S = MB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. $E_a = 0.84$ kJ mol^{-1}.	Koch68F288

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

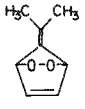
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.86.2		MeOH /*t*-BuOH (1:1) v:v	$k_r = 3.6 \times 10^7$		rt	Ad–17 A′d	S = RB, A′ = TME. Measured ($k_r/k_r^{A'}$) = 1.2. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.86.3		MeOH /*t*-BuOH (1:1) v:v	$k_r = 6.0 \times 10^7$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/NaOCl, A′ = TME. Measured ($k_r/k_r^{A'}$) = 2.0. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.86.4		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.1 \times 10^7$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A′ = TME. Measured ($k_r/k_r^{A'}$) = 0.7. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.87	6,6-dimethyl-fulvene endoperoxide 	MeOH	≈ 4.0 × 10^4	≈ 2.5	20	Od–15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 14 kJ mol^{-1}.	Koch68F288
2.88	1,5-hexadiene $CH_2=CH(CH_2)_2CH=CH_2$	CCl_4/MeOH (96:4) v:v	(2.0 ± 1.0) × 10^3		rt	A′d–8	S = MB, A′ = DPBF, ruby laser (694 nm).	Bort...77F162
2.89	*trans,trans*-2,4-hexadiene $CH_3CH=CHCH=CHCH_3$	CCl_4/MeOH (96:4) v:v	(2.0 ± 0.7) × 10^4		rt	A′d–8	S = MB, A′ = DPBF, ruby laser (694 nm).	Bort...77F162
2.90	2,5-dimethyl-2,4-hexadiene $(CH_3)_2C=CHCH=C(CH_3)_2$	MeOH	(2.0 ± 0.5) × 10^6		rt	A′d–5	S = MB, A′ = DPBF, ruby laser (694 nm).	Merk.72F260
2.90.1		MeOH	$k_r = 5.6 \times 10^6$		rt	Pa–17 P′a	S = ? A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 28.0. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662
2.90.2		CH_2Cl_2	$k_r = 1.0 \times 10^6$		rt	Pa–17 P′a	S = ? A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 5.0. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662
2.90.3		$(Me)_2CO$	$k_r = 6.4 \times 10^5$		rt	Pa–17 P′a	S = ? A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 3.2. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662
2.90.4		CH_3CN	$k_r = 1.3 \times 10^6$		rt	Pa–17 P′a	S = ? A′ = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 6.3. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

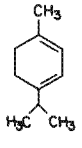
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.90.5		MeOH/H_2O (7:3)	$k_r = 5.8 \times 10^6$		rt	Pa-17 P'a	S = ? A' = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 29.0. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662
2.90.6		(Me)$_2$CO /H_2O (3:1)	$k_r = 2.6 \times 10^6$		rt	Pa-17 P'a	S = ? A' = 1-methyl-cyclohexene. Measured ($k_r/k_r^{A'}$) = 13.0. k_r derived using $k_r^{A'}$ = *2.0 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.5*].	Hast.73F662
2.91	1,3-cyclohexa-diene 	MeOH	2.2 × 10^6	4.5 × 10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 5.0 kJ mol^{-1}.	Koch68F288
2.91.1		MeOH	4.0 × 10^6	2.5 × 10^{-2}	20	Od-15	S = tetrachloroeosin. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 5.4 kJ mol^{-1}.	Koch68F288
2.91.2		MeOH	2.5 × 10^6	4.0 × 10^{-2}	20	Od-15	S = tetrachloro-fluorescein. k derived using k_d= *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 5.9 kJ mol^{-1}.	Koch68F288
2.91.3		MeOH	1.4 × 10^6	7.3 × 10^{-2}	20	Od-15	S = MB. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 5.0 kJ mol^{-1}.	Koch68F288
2.91.4		MeOH	9.1 × 10^6	1.1 × 10^{-2}	20	Od-15	S = binaphthalene-thiophene. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*]. E_a = 5.9 kJ mol^{-1}.	Koch68F288
2.91.5		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.3 \times 10^6$		rt	Ad-17 A'd	S = RB, A' = TME. Measured ($k_r^{A'}/k_r$) = 13. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.91.6		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.0 \times 10^7$		rt	Ad-17 A'd	$^1O_2$* fromH_2O_2/Ca(OCl)$_2$, A' = TME. Measured ($k_r^{A'}/k_r$) = 3. k_r derived using $k_r^{A'}$ = *3.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
2.92	α-terpinene 	MeOH	1.0 × 10^7	1.0 × 10^{-2}	15	Od-15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*I.3.6*].	Sche.58F004

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

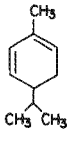
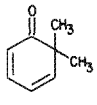
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.92.1		MeOH	3.2×10^7	3.1×10^{-3}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.7 kJ mol^{-1}.	Koch68F288
2.92.2		MeOH	3.0×10^7	3.3×10^{-3}	20	Od-15	S = tetrachloroeosin. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.3 kJ mol^{-1}.	Koch68F288
2.92.3		MeOH	1.7×10^7	6.0×10^{-3}	20	Od-15	S = tetrachloro-fluorescein. k derived using k_d= *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 0.84 kJ mol^{-1}.	Koch68F288
2.92.4		MeOH	2.5×10^7	4.0×10^{-3}	20	Od-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.7 kJ mol^{-1}.	Koch68F288
2.92.5		MeOH	7.1×10^7	1.4×10^{-3}	20	Od-15	S = binaphthalene-thiophene. k derived using k_d= *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.3 kJ mol^{-1}.	Koch68F288
2.92.6		MeOH	7.7×10^7	1.3×10^{-3}	20	Od-15	S = acridine orange. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.7 kJ mol^{-1}.	Koch68F288
2.93	α-phellandrene 	MeOH	1.0×10^7	1.0×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 4.2 kJ mol^{-1}.	Koch68F288
2.94	2,2-dimethyl-cyclohexa-3,5-diene-1-one 	MeOH	$\approx 5.3 \times 10^4$	≈ 1.9	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*] E_a = 15 kJ mol^{-1}.	Koch68F288
2.94a	2-methylnorborna-2,5-diene 	CH_3CN	$k_r = 1.2 \times 10^5$		0	Ad-17 A'd	S = MB, A' = 2-methyl-idenenorborn-5-ene. Measured ($k_r/k_r^{A'}$) = 34.0. k_r derived using $k_r^{A'} = 3.6 \times 10^3$ dm^3 mol^{-1} s^{-1} [*2.94b*].	Jeff.78F149
2.94b	2-methylidene-norborn-5-ene 	CH_3CN	$k_r = 3.6 \times 10^3$		0	Ad-17 A'd	S = MB, A' = 1-methyl-cyclopentene. Measured ($k_r^{A'}/k_r$) = 507. k_r derived using $k_r^{A'}$ = *1.8×10^6 dm^3 mol^{-1} s^{-1} [*A3.4*].	Jeff.78F149

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

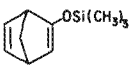
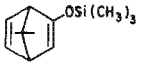
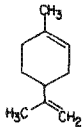
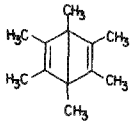
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.95	2-(trimethylsiloxy)norborna-2,5-diene 	$CDCl_3$	$(k_r/k_r^{A'}) = 1.7 \times 10^{-1}$		rt	Ad-17 A'd	S = *meso*-TPP, A' = 7,7-dimethyl-2-(trimethylsiloxy)norborn-2-ene.	Jeff.78F290
2.96	7,7-dimethyl-2-(trimethylsiloxy)-norborna-2,5-diene 	$CDCl_3$	$(k_r/k_r^{A'}) = 4.2$		rt	Ad-17 A'd	S = *meso*-TPP, A' = 7,7-dimethyl-2-(trimethylsiloxy)norborn-2-ene.	Jeff.78F290
2.97	limonene 	MeOH(?)	5.9×10^4	1.7	rt	?	Method not given. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Goll62F005
2.97.1		MeOH	5.9×10^4	1.7	20	Od-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 8.4 kJ mol^{-1}.	Koch68F288
2.98	nopadiene 	MeOH	$\approx 5.0 \times 10^4$	≈ 2.0	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 16 kJ mol^{-1}.	Koch68F288
2.99	hexamethylbicyclo[2.2.0]-hexa-2,5-diene 	$CHCl_3$	$(1.1 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
2.100	2,7-dimethyl-7-hydroperoxy-2,5-octadiene $(CH_3)_2C(OOH)CH=CHCH_2CH=C(CH_3)_2$	MeOH	k(total) = 4.2×10^5 $k(P_1) = 1.9 \times 10^5$ $k(P_2) = 2.3 \times 10^5$	2.7×10^{-1}	-20	Od 14 Pa-Ad 27	S = RB, A' = α-terpinene, P_1 = 2,7-dimethyl-2,7-dihydroperoxide-3,5-octadiene, P_2 = 2,7-dimethyl-2,6-dihydroperoxide-3,7-octadiene. k derived using k_d = 1.1×10^5 s^{-1} [*1.3.4*].	Tani.78A357
2.101	3,7-dimethyl-1,6-octadiene-2-ol $(CH_3)_2C=CH(CH_2)_2C(CH_3)C(OH)=CH_2$	MeOH	$(k_r^{A'}/k_r) = 7.3 \times 10^{-2}$		rt	Ad-17 A'd	S = RB, A' = 2,6-di-*t*-butylphenol.	Mats...72F520
2.101.1		CH_2Cl_2	$(k_r^{A'}/k_r) = 4.2 \times 10^{-2}$		rt	Ad-17 A'd	$^1O_2$* from $(PhO)_3PO_3$ decomposition, A' = 2,6-di-*t*-butylphenol.	Mats...72F520

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

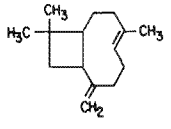
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.102	*cis*-2,6-dimethyl-2,6-octadiene $CH_3CH=C(CH_3)(CH_2)_2CH=C(CH_3)_2$	MeOH	1.11×10^6		-20	Od-14 27	S = RB, A' = α-terpinene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A344
2.103	*trans*-2,6-dimethyl-2,6-octadiene $CH_3CH=C(CH_3)(CH_2)_2CH=C(CH_3)_2$	MeOH	1.85×10^6		-20	Od-14 27	S = RB, A' = α-terpinene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A344
2.104	mixture of all monohydroperoxides obtained from photosensitized oxygenation of *trans*-2,6-dimethyl-2,6-octadiene.	MeOH	7.4×10^5		-20	Od 14 Ad-Pa 27	S = RB, A' = α-terpinene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A344
2.105	2,7-dimethyl-2,6-octadiene $(CH_3)_2C=CH(CH_2)_2CH=C(CH_3)_2$	MeOH	k(total) = 1.7×10^6 $k(P_1) = 9.0 \times 10^5$ $k(P_2) = 8.1 \times 10^5$	6.5×10^{-2}	-20	Od 14 Pa-Ad 27	S = RB, A' = α-terpinene. P_1 = 2,7-dimethyl-7-hydroperoxide-2,5-octadiene, P_2 = 2,7-dimethyl-6-hydroperoxide-2,7-octadiene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A357
2.106	2,7-dimethyl-6-hydroperoxy-2,7-octadiene $CH_2=C(CH_3)CH(OOH)(CH_2)_2CH=C(CH_3)_2$	MeOH	k(total) = 6.0×10^5 $k(P_1) = 1.9 \times 10^5$ $k(P_2) = 4.1 \times 10^5$	1.9×10^{-1}	-20	Od 14 Pa-Ad 27	S = RB, A' = α-terpinene. P_1 = 2,7-dimethyl-2,6-dihydroperoxide-3,7-octadiene, P_2 = 2,7-dimethyl-3,6-dihydroperoxide-1,7-octadiene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A357
2.107	*trans*-2,6,9-trimethyl-1,6-decadiene $(CH_3)_2CHCH_2CH=C(CH_3)(CH_2)_3C(CH_3)=CH_2$	EtOH /*i*-PrOH (1:1) v:v	8.4×10^5 (est)	8.0×10^{-2}	19	Od-14 27	S = RB, A' = DMF. *k* estimated using $k_d = 6.7 \times 10^4$ s^{-1} (calc).	Schu..78F464
2.108	*cis*-2,6,9-trimethyl-1,6-decadiene $(CH_3)_2CHCH_2CH=C(CH_3)(CH_2)_3C(CH_3)=CH_2$	EtOH /*i*-PrOH (1:1) v:v	6.1×10^5 (est)	1.1×10^{-1}	19	Od-14 27	S = RB, A' = DMF. *k* estimated using $k_d = 6.7 \times 10^4$ s^{-1} (calc).	Schu..78F464
2.109	*trans*-2,6-dimethyl-1,6-undecadiene $CH_3(CH_2)_3CH=C(CH_3)(CH_2)_3C(CH_3)=CH_2$	EtOH /*i*-PrOH (1:1) v:v	6.7×10^5 (est)	1.0×10^{-1}	19	Od-14 27	S = RB, A' = DMF. *k* estimated using $k_d = 6.7 \times 10^4$ s^{-1} (calc).	Schu..78F464
2.110	*cis*-2,6-dimethyl-1,6-undecadiene $CH_3(CH_2)_3CH=C(CH_3)(CH_2)_3C(CH_3)=CH_2$	EtOH /*i*-PrOH (1:1) v:v	5.2×10^5 (est)	1.3×10^{-1}	19	Od-14 27	S = RB, A' = DMF. *k* estimated using $k_d = 6.7 \times 10^4$ s^{-1} (calc).	Schu..78F464
2.111	(-)-caryophyllene 	MeOH /C_6H_6 (1:1) v:v	(k_r/k_r') = 5.1		20	Ad-17 A'd	S = BP, triphenylene, quinoline,Naph,Py, RB,MB; A' = (-)-isocaryophyllene.	Goll...70F735
2.112	*trans-trans*-4,8-dimethyl-4,8-dodecadiene $CH_3(CH_2)_2CH=C(CH_3)(CH_2)_2CH=C(CH_3)(CH_2)_2CH_3$	MeOH	1.11×10^6		-20	Od-14 27	S = RB, A' = α-terpinene. *k* derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*].	Tani.78A344

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

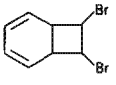
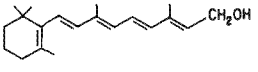
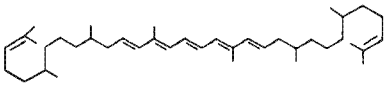
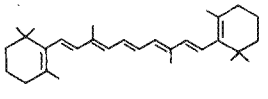
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.113	4,8-dimethyl-4,8-dodecadiene (*cis-cis:cis-trans* + *trans-cis:trans-trans*) 24:52:24	MeOH	6.94×10^5		-20	Od-14 27	S = RB, A′ = α-terpinene. k derived using k_d = 1.1×10^5 s^{-1} [*1.3.4*].	Tani.78A344
2.114	mixture of all monohydroperoxides obtained from photosensitized oxygenation 4,8-dimethyl-4,8-dodecadiene	MeOH	3.82×10^5		-20	Od 14 Ad-Pa 27	S = RB, A′ = α-terpinene. k derived using k_d = 1.1×10^5 s^{-1} [*1.3.4*].	Tani.78A344
2.115	6,6-dimethylfulvene 	MeOH	1.7×10^7	6.0×10^{-3}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 1.3 kJ mol^{-1}.	Koch68F288
2.116	alloocimine-A $CH_3CH=C(CH_3)CH=CHCH=C(CH_3)_2$	MeOH	1.4×10^6	7.0×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 8.4 kJ mol^{-1}.	Koch68F288
2.117	cyclooctatetraene dibromide 	MeOH	$\approx 3.3 \times 10^5$	$\approx 3.0 \times 10^{-1}$	20	Od-15	S = RB. k derived using k_d = *1.0×10^5. s^{-1} [*1.3.6*]. E_a = 11 kJ mol^{-1}.	Koch68F288
2.118	sarcina phytoene (3 conj. bonds)	C_6H_6/MeOH (3:2) v:v	$\leqslant 1.9 \times 10^7$ (est)	$\geqslant 5.3 \times 10^{-3}$	rt	A′d-22	S = MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042
2.119	all *trans*-retinol 	C_6H_6/MeOH (4:1) v:v	$< 7.3 \times 10^6$		rt	Pa-20	S = MB, A′ = 2M2P. Measured ($k/k_{A'}$) $\leqslant$ 9. k derived using $k_{A'}$ = *8.1×10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot...70F188
2.120	sarcina phytofluene 	C_6H_6/MeOH (3:2) v:v	$\leqslant 1.0 \times 10^8$ (est)	$\geqslant 1.0 \times 10^{-3}$	rt	A′d-22	S = MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042
2.121	C-30 carotene analog 	C_6H_6/MeOH (4:1) v:v	4.6×10^7		rt	Pa-20	S = MB, A′ = 2M2P. Measured ($k/k_{A'}$) = (57 ± 86). k derived using $k_{A'}$ = *8.1×10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot..70F188
2.122	P-422 (8 conj. bonds)	C_6H_6/MeOH (3:2) v:v	1.2×10^{10} (est)	8.3×10^{-6}	rt	A′d-22	S = MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

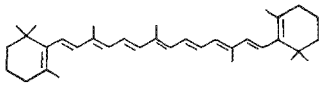
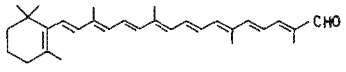
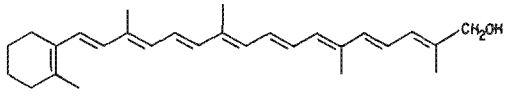
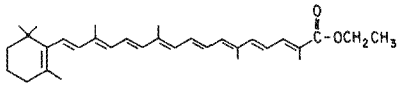
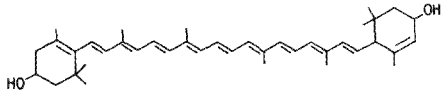
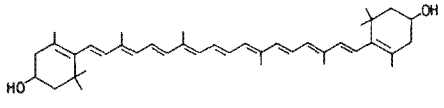
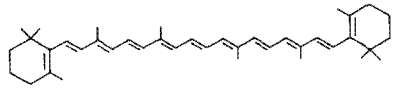
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.123	C-35 carotene analog 	C_6H_6/MeOH (4:1) v:v	1.5×10^9		rt	Pa-20	S = MB, A′ = 2M2P. Measured ($k/k_{A'}$) = (1900 ± 2850). k derived using $k_{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot..70F188
2.124	P-438 (probably sarcina-xanthin-9 conj. bonds)	C_6H_6/MeOH (3:2) v:v (est)	3.1×10^{10}	3.2×10^{-6}	rt	A′d-22	S = MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042
2.125	β-apo-8′-carotenal 	C_6H_6	$(1.4 \pm 0.2) \times 10^{10}$		rt	Ad-12	S = An, ruby laser (347 nm).	Wilk.78F276
2.126	β-apo-8′-carotenol 	C_6H_6/MeOH (4:1) v:v	$\approx 1.5 \times 10^9$		rt	P′a-20	S = MB, A′ = 2M2P. Measured ($k/k_{A'}$) ≈ 1900. k derived using $k_{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot..70F188
2.126.1		C_6H_6/MeOH (4:1) v:v	1.2×10^{10}		25	P′a-20	S= MB, A′ = 2M2P. Measured ($k/k_{A'}$) ≈ 1.5×10^4. k derived using $k_{A'}$ = *8.1 × 10^5 dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot....70F734
2.127	ethyl-β-apo-8′-carotenoate 	C_6H_6	$(1.2 \pm 0.2) \times 10^{10}$		rt	Ad-12	S = An, ruby laser (347 nm).	Wilk.78F276
2.128	lutein 	C_6H_6/MeOH (3:2) v:v (est)	2.1×10^{10}	4.8×10^{-6}	rt	A′d-22	S = MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042
2.129	isozeaxanthin 	C_6H_6/MeOH (3:2) v:v (est)	2.9×10^{10}	3.4×10^{-6}	rt	A′d-22	S =MB, A′ = Rub. k estimated using k_d = 1.0×10^5 s^{-1} (calc).	Math...74F042
2.130	β-carotene Car 	MeOH	1.6×10^{10}	$(6.1 \pm 0.6) \times 10^{-6}$	rt	A′d-16	S = RB, A′ = DPF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn..71F398
2.130.1		CCl_4	$(7.0 \pm 2.1) \times 10^9$		rt	Ld-13	S = ? k derived using k_d = 3.5×10^1 s^{-1} [*1.8.3*].	Kras79A010

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.130.2	CH_2Cl_2	8.5×10^9 (est)		rt	A'd-23	S = A' = Rub. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl..73P066
2.130.3	CH_2Cl_2	1.3×10^{10} (est)		25	A'd-23	S = A' = Rub. k estimated using $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 8.0 \times 10^3$ s^{-1}.	Carl..74F341
2.130.4	CH_2Cl_2	1.7×10^{10}		30	Od-23	S = MB, A' = TME. k derived using $k_{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*] and $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Taim.76F901
2.130.5	CH_2Cl_2	4.4×10^9		30	Od-23	S = MB, A' = 1,3-cyclohexadiene. k derived using $k_{A'} = *3.5 \times 10^6$ dm^3 mol^{-1} s^{-1} [*A3.8*] and $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Taim.76F921
2.130.6	CH_2Cl_2	1.9×10^{10}		30	Od-23	S = MB, A' = Rub. k derived using $k_{A'} = *4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.14*] and $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Taim.76F921
2.130.7	CS_2	3.3×10^{10}	1.5×10^{-7}	rt	P'a-20	S = TPP, A' = 2M2P. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Foot..72F028
2.130.8	$CFCl_2$–CF_2Cl	1.4×10^9		rt	Ad-36	$^1O_2$* from Nd/YAG laser (1065 nm). Measured $(k/k_{O_2}) = (1.1 \pm 0.2) \times 10^6$. k derived using $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value).	Math.72M077
2.130.9	*n*-BuOH	9.5×10^9	$(5.5 \pm 0.6) \times 10^{-6}$	rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Youn..71F398
2.130.10	*t*-BuOH	7.9×10^9	$(3.8 \pm 0.4) \times 10^{-6}$	rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Youn..71F398
2.130.11	C_5H_5N	6.5×10^9		rt	A'd-23	S = A' = Rub. k derived using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = *6.0 \times 10^4$ s^{-1} [*1.29.1*].	Fahr...74R112
2.130.12	C_6H_6	$(1.3 \pm 0.2) \times 10^{10}$		25	A'd-8	S = An, A' = DPBF, ruby laser (694 nm).	Farm.73F438
2.130.13	C_6H_6	$(2.0 \pm 0.5) \times 10^{10}$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm). Solvent contained 2% MeOH.	Merk.72F260
2.130.14	C_6H_6	$(1.1 \pm 0.1) \times 10^{10}$		25	Ad-12	S = An, ruby laser (347 nm).	Farm.73F438
2.130.15	C_6H_6	$(1.25 \pm 0.2) \times 10^{10}$		rt	Ad-12	S = An, ruby laser (347 nm).	Wilk.78F276

TABLE 2. Rate constants for the interaction of singlet oxygen with olefinic substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
2.130.16		C_6H_5Br	3.4×10^9 (est)		0	A'd-33	$^1O_2$* from microwave discharge, A' = Rub. Measured $k/[(k_d/[A']) + k_{A'}] = 33.7$ at $[A'] = 1.5 \times 10^{-4}$ mol dm^{-3}. k estimated using $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*] and $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Guil.73F333
2.130.17		$C_6H_5CH_3$	3.0×10^{10} (est)		rt	A'd-25	S = A' = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_{A'} = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
2.130.18		CCl_4 /$CHCl_3$ (9:1) v:v	6.2×10^9 (est)		rt	A'd-23	S = A' = Rub. Measured $k/(k_{A'}[A'] + k_d) = 3.5 \times 10^6$ dm^3 mol^{-1} at $[A'] = 5 \times 10^{-6}$ mol dm^{-3}. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
2.130.18a		EtOH/H_2O (95:5) v:v	$(2.2 \pm 0.5) \times 10^9$		rt	Ld-13	$^1O_2$* from pyrogallol autooxidation by O_2/KOH. k measured by monitoring the quenching of chemiluminescence by A.	Slaw78F605
2.130.19		C_6H_6/MeOH (4:1) v:v	1.2×10^{10}		25	P'a-20	S = MB, A' = 2M2P. Measured $(k/k_{A'}) = 1.5 \times 10^4$. k derived using $k_{A'} = *8.1 \times 10^5$ dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot....70F734
2.130.20		C_6H_6/MeOH (4:1) v:v	9.7×10^9	$(3.9 \pm 0.4) \times 10^{-6}$	rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 3.8 \times 10^4$ s^{-1} [*1.49*].	Youn..71F398
2.130.21		C_6H_6/MeOH (3:2) v:v	2.3×10^{10} (est)	4.3×10^{-6}	rt	A'd-22	S = MB, A' = Rub. k estimated using $k_d = 1.0 \times 10^5$ s^{-1} (calc).	Math...74F042
2.130.22		C_6H_6/EtOH (8:1) v:v	1.3×10^{10} (est)		22	P'a-13	S = RB, A' = TMHP, P' = nitroxy radicals. k estimated using $k_d = 3 \times 10^4$ s^{-1} (calc).	Ivan....75F445
2.130.23		C_6H_6/EtOH (2:1) v:v	1.65×10^{10} (est)		rt	A'd-19	S = RB, A' = chlorophyll-a. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
		For more relative rates see		2.55, 4.7.6.				
2.131	canthaxanthin	C_6H_6	$(1.45 \pm 0.2) \times 10^{10}$		rt	Ad-12	S = An, ruby laser (347 nm).	Wilk.78F276
2.132	lycopene	C_6H_6/MeOH (4:1) v:v	$\approx 1.2 \times 10^{10}$		rt	P'a-20	S = MB, A' 2M2P. Measured $(k/k_{A'}) = 1.5 \times 10^4$. k derived using $k_{A'} = *8.1 \times 10^5$ dm^3 mol^{-1} s^{-1} [*A3.3*].	Foot.70F188

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons

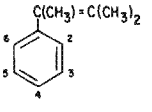
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
3.1	benzene C_6H_6	CCl_4	$(2.2 \pm 1.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
3.1.1		CCl_4/MeOH (96:4) v:v	$(5.0 \pm 3.0) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.2	bromobenzene C_6H_5Br	CCl_4	$(1.9 \pm 1.3) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
3.3	ethylbenzene $C_6H_5C_2H_5$	CCl_4/MeOH (96:4) v:v	$(5.0 \pm 3.0) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.4	methoxybenzene $C_6H_5OCH_3$	MeOH	$k_r \leqslant 5 \times 10^6$ (est)		20	Ad-17 A'd	S = RB, and MB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.5	methyl benzoate $C_6H_5COOCH_3$	CCl_4	$(2.9 \pm 1.8) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
3.6	styrene $C_6H_5CH=CH_2$	CCl_4/MeOH (96:4) v:v	$(5.0 \pm 2.0) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.7	*cis*-β-methyl-styrene $C_6H_5CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(5.0 \pm 1.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.8	*trans*-β-methyl-styrene $C_6H_5CH=CHCH_3$	CCl_4/MeOH (96:4) v:v	$(2.0 \pm 1.0) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort.77F162
3.9	3-methyl-1-phenyl-2-butene $C_6H_5CH_2CH=C(CH_3)_2$	MeOH(?)	7.7×10^5	1.3×10^{-1}	rt	?	Method not given. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Goll62F005
3.9.1		MeOH	6.7×10^5	1.5×10^{-1}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. $E_a = 9.6$ kJ mol^{-1}.	Koch68F288
		COMPOUNDS 3.10 - 3.19 : 						
3.10	trimethylstyrene (TMS)	MeOH /C_5H_5N (98:2) v:v	$k_r = 5.0 \times 10^6$		rt	Pa-17 P'a	S= RB, A' = *p*-methoxy-trimethstyrene. Measured ($k_r/k_r^{A'}$) = 0.51. k_r derived using $k_r^{A'} = 9.9 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.18*].	Foot.71F577
3.10.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 4.8 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methoxytrimethyl-styrene. Measured. ($k_r/k_r^{A'}$) = 0.57. k_r derived using $k_r^{A'} = 8.4 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.18.1*].	Foot.71F577
3.10.2		MeOH /*t*-BuOH (1:1) v:v	$k_r = 5.2 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methyltrimethylstyrene. Measured ($k_r^{A'}/k_r$) = 1.20. k_r derived using $k_r^{A'} = 6.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577
		For more relative rates see		2.19, 2.19.1-5.				

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.11	*m*-chlorotrimethylstyrene [R_3 = -Cl]	MeOH /C_5H_5N (98:2) v:v	$k_r = 2.8 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.384. k_r derived using $k_r^{A'} = 7.2 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13*].	Foot.71F577
3.11.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.7 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.436. k_r derived using $k_r^{A'} = 6.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577
3.12	*p*-chlorotrimethylstyrene [R_4 = -Cl]	MeOH	$k_r = 3.3 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = 2-methyl-2-butene. Measured ($k_r/k_r^{A'}$) = 2.23. k_r derived using $k_r^{A'}$ = *1.5 $\times 10^6$ dm^3 mol^{-1} s^{-1} [*A3.1*].	Foot.71F577
		For more relative rates see		3.13, 3.13.1, 3.14, 3.14.1.				
3.13	*p*-methyltrimethylstyrene [R_4 = -Me]	MeOH /C_5H_5N (98:2) v:v	$k_r = 7.2 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-clorotrimethylstyrene. Measured ($k_r^{A'}/k_r$) = 0.457. k_r derived using $k_r^{A'} = 3.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.12*].	Foot.71F577
3.13.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 6.3 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-chlorotrimethylstyrene. Measured ($k_r^{A'}/k_r$) = 0.526. k_r derived using $k_r^{A'}$ = 3.3×10^6 dm^3 mol^{-1} s^{-1} [*3.12*].	Foot.71F577
		For more relative rates see		3.10.2, 3.11, 3.11.1, 3.15, 3.16, 3.16.1, 3.17, 3.17.1, 3.18, 3.18.1.				
3.14	*m*-methyltrimethylstyrene [R_3 = -Me]	MeOH /C_5H_5N (98:2) v:v	$k_r = 5.1 \times 10^6$		rt	Pa-17 P'a	S =RB, A' = *p*-chlorotrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 1.54. k_r derived using $k_r^{A'} = 3.3 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.12*].	Foot.71F577
3.14.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 4.7 \times 10^9$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-chlorotrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 1.43. k_r derived using $k_r^{A'}$ = 3.3×10^6 dm^3 mol^{-1} s^{-1} [*3.12*].	Foot.71F577
3.15	*m*-cyanotrimethylstyrene [R_3 = -CN]	MeOH /C_5H_5N (98:2) v:v	$k_r = 1.4 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.197. k_r derived using $k_r^{A'} = 7.2 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13*].	Foot.71F577
3.15.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.6 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.252. k_r derived using $k_r^{A'}$ = 6.3×10^6 dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

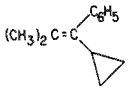
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.16	*p*-cyanotrimethylstyrene [R_4 = -CN]	MeOH /*t*-BuOH (98:2) v:v	$k_r = 1.2 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.172. k_r derived using $k_r^{A'} = 7.2 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13*].	Foot.71F577
3.16.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 9.7 \times 10^5$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.154. k_r derived using $k_r^{A'}$ = 6.3×10^6 dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577
3.17	*m*-methoxytrimethylstyrene [R_3 = -OMe]	MeOH /C_5H_5N (98:2) v:v	$k_r = 4.8 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.667. k_r derived using $k_r^{A'} = 7.2 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13*].	Foot.71F577
3.17.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 5.2 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 0.721. k_r derived using $k_r^{A'}$ = 6.3×10^6 dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577
3.18	*p*-methoxytrimethylstyrene [R_4 = -OMe]	MeOH /C_5H_5N (98:2) v:v	$k_r = 9.9 \times 10^6$		rt	Pa-17 P'a	S = RB, A' = *p*-methyltrimethylstryene. Measured ($k_r/k_r^{A'}$) = 1.38. k_r derived using $k_r^{A'} = 7.2 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.13*].	Foot.71F577
3.18.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 8.4 \times 10^6$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methyltrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 1.33. k_r derived using $k_r^{A'}$ = 6.3×10^6 dm^3 mol^{-1} s^{-1} [*3.13.1*].	Foot.71F577
		For more relative rates see		3.10, 3.10.1, 3.19, 3.19.1.				
3.19	*p*-(*N*,*N*-dimethylamino)trimethylstyrene [R_4 = -N(CH$_3$)$_2$]	MeOH /C_5H_5N (98:2) v:v	$k_r = 2.0 \times 10^7$		rt	Pa-17 P'a	S = RB, A' = *p*-methoxytrimethylstryene. Measured ($k_r/k_r^{A'}$) = 2.0. k_r derived using $k_r^{A'} = 9.9 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.18*].	Foot.71F577
3.19.1		MeOH /*t*-BuOH (1:1) v:v	$k_r = 2.4 \times 10^7$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = *p*-methoxytrimethylstyrene. Measured ($k_r/k_r^{A'}$) = 2.9. k_r derived using $k_r^{A'}$ = 8.4×10^6 dm^3 mol^{-1} s^{-1} [*3.18.1*].	Foot.71F577
3.20	1-cyclopropyl-2-methyl-1-phenylpropene 	$(Me)_2CO$	$k_r = 1.2 \times 10^6$		rt	Ad-17 A'd	S = Eos, A' = (dicyclopropylmethylidene cyclobutane. Measured ($k_r/k_r^{A'}$) = 0.79. k_r derived using $k_r^{A'}$ = 1.5×10^6 dm^3 mol^{-1} s^{-1} [*2.19.4*].	Rous..78F430

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

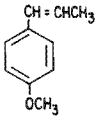
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.21	*cis*-stilbene $C_6H_5CH=CHC_6H_5$	CCl_4/MeOH (96:4) v:v	$(3.0 \pm 1.5) \times 10^3$		rt	A'd-8	A = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.22	*cis*-α-methyl-stilbene $C_6H_5C(CH_3)=CHC_6H_5$	CCl_4/MeOH (96:4) v:v	$(6.0 \pm 2.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.23	*trans*-α-methyl-stilbene $C_6H_5C(CH_3)=CHC_6H_5$	CCl_4/MeOH (96:4) v:v	$(3.0 \pm 1.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
3.24	1,2-dimethoxy-stilbene $C_6H_5C(OCH_3)=C(OCH_3)C_6H_5$	$(Me)_2CO$	$k_r = 9.7 \times 10^6$ *7.9×10^6		8	?	S = ?, A' = *p*-dioxene. Measured ($k_r/k_r^{A'}$) = 44. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
3.25	1,2-dimethoxy-benzene 1,2-$C_6H_4(OCH_3)_2$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = RB and MB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.26	1,3-dimethoxy-benzene 1,3-$C_6H_4(OCH_3)_2$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.27	1,4-dimethoxy-benzene 1,4-$C_6H_4(OCH_3)_2$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.28	anethole 	MeOH	$\approx 1.0 \times 10^7$	$\approx 1.0 \times 10^{-2}$	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 17 kJ mol^{-1}.	Koch68F288
3.29	1,2,3-trimethoxy-benzene 1,2,3-$C_6H_3(OCH_3)_3$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.30	1,2,4-trimethoxy-benzene 1,2,4-$C_6H_3(OCH_3)_3$	MeOH	1.80×10^7	6.44×10^{-3}	rt	A'd-16	S = MB, A' = DPF. k derived using k_d = 1.16×10^5 s^{-1} ([*1.3*];[*1.3.2*]; [*1.3.3*])[a].	Thom.78A171
		For more relative rates see		3.34.				
3.31	1,3,5-trimethoxy-benzene 1,3,5-$C_6H_3(OCH_3)_3$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.32	1,2,3,4-tetra-methoxybenzene 1,2,3,4-$C_6H_2(OCH_3)_4$	MeOH	$k_r \leq 5 \times 10^6$ (est)		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect.	Sait..72A020
3.33	1,2,3,5-tetra-methoxybenzene 1,2,3,5-$C_6H_2(OCH_3)_4$	MeOH	$k_r = 3.1 \times 10^7$		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. Measured ($k_r/k_r^{A'}$) = 0.148. k_r derived using $k_r^{A'}$ = 2.1×10^8 dm^3 mol^{-1} s^{-1} [*3.34*]. k_r is a mean for runs using both S.	Sait..72A020

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

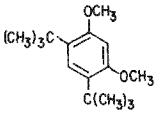
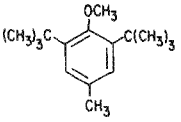
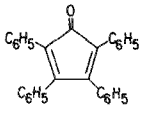
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_q/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.34	1,2,4,5-tetra-methoxybenzene 1,2,4,5-$C_6H_2(OCH_3)_4$	MeOH	$k_r = 2.1 \times 10^8$		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4-trimethoxy benzene. Measured ($k_r/k_r^{A'}$) = 11.6. k_r derived using $k_r^{A'}$ = 1.8×10^7 dm^3 mol^{-1} s^{-1} [*3.30*]. k is a mean for runs using both S.	Sait..72A020
		For more relative rates see		3.25-7, 3.29, 3.31-3, 3.37, 3.39.				
3.35	1,3-dimethoxy-4,6-di-*t*-butyl benzene 	MeOH(?)	$k_r = 7.0 \times 10^4$		rt	Pa-17 P'a	S = RB, A' = TME. Measured ($k_r/k_r^{A'}$) = 2.3×10^{-3}. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Sait..70F454
3.35.1		MeOH(?)	$k_r = 9.0 \times 10^4$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = TME. Measured ($k_r/k_r^{A'}$) = 3.0×10^{-3}. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Sait..70F454
3.36	2,6-di-*t*-butyl-4-methylanisole 	MeOH	5.9×10^5	2.0×10^{-1}	rt	A'd-16	S = MB, A' = DPF. k derived using k_d = 1.16×10^5 s^{-1} ([*1.3*]; [*1.3.2*];[*1.3.3*])[a].	Thom.78A171
3.37	pentamethoxy-benzene 1,2,3,4,5-$C_6H(OCH_3)_5$	MeOH	$k_r = 4.1 \times 10^7$		20	Ad-17 A'd	S - MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. Measured ($k_r k_r^{A'}$) = 0.193. k_r derived using $k_r^{A'}$ = 2.1×10^8 dm^3 mol^{-1} s^{-1} [*3.34*]. k is a mean for runs using both S.	Sait..72A020
3.38	tetraphenylcyclo-pentadienone 	CCl_2F-$CClF_2$	8.9×10^6 $k_r = 3.3 \times 10^6$ $k_q = 5.6 \times 10^6$	5.3×10^{-5}	25	Ad-34	$^1O_2$* from Nd-YAG laser (1065 nm), A' = DPBF. Measured (k_q/k_r) = 1.7. k, k_r, and k_q derived using k_d = 4.7×10^2 s^{-1} ([*1(a).2*]; [*1(a).2.1*])[a].	Evan.76F417
3.38.1		CCl_2F-$CClF_2$	$k_r = 2.8 \times 10^6$ (est)		rt	Ad-36	$^1O_2$* directly from CW Nd-YAG laser (1065 nm). Measured ($k_r/k_{O_2}[O_2]$) = 700 dm^3 mol^{-1}. k_r estimated using $k_{O_2}[O_2] = 4 \times 10^3$ s^{-1} (based on gas phase value of $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1}).	Math.70F387

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

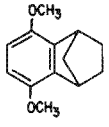
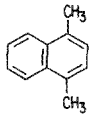
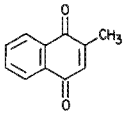
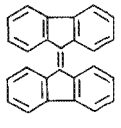
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.39	hexamethoxy-benzene 1,2,3,4,5,6-$C_6(OCH_3)_6$	MeOH	$k_r = 6.5 \times 10^6$		20	Ad-17 A'd	S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. Measured $(k_r/k_r^{A'}) = 3.1 \times 10^{-2}$. k_r derived using $k_r^{A'} = 2.1 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.34*]. k_r is a mean for runs using both S.	Sait..72A020
3.39a	1,4-dimethoxy-benzonorbornene 	C_6H_6 /MeOH (3:1) v:v	6×10^6		25	A'd-20	S = RB, A' = cyclohexene. k derived using $\beta_{A'} = 3.1$ mol^{-1} dm^{-3} [*2.54.3*] and $k_d = 6.25 \times 10^4$ s^{-1}.	Kret.78F586
3.40	indene 	MeOH	6.7×10^4	1.5	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*] $E_a = 13$ kJ mol^{-1}.	Koch68F288
3.40.1		MeOH	5.0×10^4	2.0	20	Od-15	S = MB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. $E_a = 11$ kJ mol^{-1}.	Koch68F288
3.41	1,4-dimethyl-naphthalene 	C_6H_{12}	$k_r = 1.2 \times 10^4$		25	Ad-17 A'd	S = A' = An. Measured $(k_r/k_r^{A'}) = 7.5 \times 10^{-2}$. k_r derived using $k_r^{A'} = 1.6 \times 10^5$ dm^3 mol^{-1} s^{-1} [*3.44.9*].	Stev..74F312
3.42	2-methyl-1,4-naphthalendione 	EtOH	2.37×10^6 (est)		rt	A'd-19	S = RB, A' = chloro-phyll-a. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
3.43	9,9'-bifluorenyl-idene 	CH_2Cl_2	$k_r = 1.0 \times 10^6$		rt	Ad-17 A'd	S = MB, A' = TME. Measured $(k_r/k_r^{A'}) = 3.4 \times 10^{-2}$. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Rich.70F200
3.43.1		dioxane /MeOH (4:1) v:v	$k_r = 1.0 \times 10^6$		rt	Ad-17 A'd	$^1O_2$* from H_2O_2/NaOCl, A' = TME. Measured $(k_r/k_r^{A'}) = 3.4 \times 10^{-2}$. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Rich.70F200

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

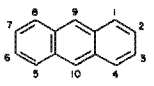
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
			COMPOUNDS 3.44 - 3.59 :					
								
3.44	anthracene (An)	$CHCl_3$	7.4×10^5	1.36×10^{-2}	rt	Od-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe53F004
3.44.1		$CHCl_3$	2.8×10^5	3.6×10^{-2}	rt	Pa-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe55F004
3.44.2		$CHCl_3$	$(5.4 \pm 0.6) \times 10^5$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
3.44.3		CCl_4	4.25×10^5	4.0×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.7×10^3 s^{-1} [*1.8.4*].	Bowe53F004
3.44.4		CS_2	1.4×10^6	3.6×10^{-3}	rt	Od-15	S = self. k derived using k_d = 5.0×10^3 s^{-1} [*1.9*].	Bowe53F004
3.44.5		CS_2	1.9×10^6	2.6×10^{-3}	rt	Ad-15	S = DNT. k derived using k_d = 5.0×10^3 s^{-1} [*1.9*].	Foot..72F028
3.44.6		C_6H_6	9.5×10^4	4.2×10^{-1}	rt	Pa-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Bowe.55F004
3.44.7		C_6H_6	7.0×10^4	5.7×10^{-1}	rt	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Livi.59F003
3.44.8		C_6H_6	8.5×10^5	4.7×10^{-2}	rt	Ad-15	S = DNT. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Foot..72F028
3.44.9		C_6H_6	1.6×10^5	$(2.7 \pm 0.5) \times 10^{-1}$	25	A'd-20	S = A' = Rub. k derived using $\beta_{A'}$ = 1.0×10^{-3} mol dm^{-3} [*3.63.18*] and k_d = 4.2×10^4 s^{-1} [*1.32*].	Stev..74F312
3.44.10		C_6H_5Br	1.1×10^5	1.2×10^{-1}	rt	Ad-15	S = self. k derived using k_d = 1.3×10^4 s^{-1} [*1.34*].	Livi.59F003
3.44.11		CS_2/C_6H_6 (99:1) Mole %	3.3×10^5 (est)	1.5×10^{-2}	rt	Od-15	S = self. k estimated using k_d = 5.0×10^3 s^{-1} (calc).	Bowe53F004
3.44.12		CS_2/C_6H_6 (95:5) Mole %	1.6×10^5 (est)	3.8×10^{-2}	rt	Od-15	S = self. k estimated using k_d = 6.2×10^3 s^{-1} (calc).	Bowe53F004
3.44.13		CS_2/C_6H_6 (90:10) Mole %	1.2×10^5 (est)	6.2×10^{-2}	rt	Od-15	S = self. k estimated using k_d = 7.5×10^3 s^{-1} (calc).	Bowe53F004
3.44.14		CS_2/C_6H_6 (96:4) Mole %	2.4×10^5 (est)	2.7×10^{-2}	rt	Ad-15	S = DNT. k estimated using k_d = 6.4×10^3 s^{-1} (calc).	Foot..72F028
3.44.15		CS_2/C_6H_6 (93:7) Mole %	1.4×10^5 (est)	5.2×10^{-2}	rt	Ad-15	S = DNT. k estimated using k_d = 7.5×10^3 s^{-1} (calc).	Foot..72F028
3.44.16		CS_2/C_6H_6 (75:25) Mole %	1.5×10^5 (est)	9.4×10^{-2}	rt	Ad-15	S = TPP. k estimated using k_d = 1.4×10^4 s^{-1} (calc).	Foot..72F028
3.44.17		CS_2/C_6H_6 (50:50) Mole %	3.0×10^5 (est)	7.7×10^{-2}	rt	Ad-15	S = TPP. k estimated using k_d = 2.3×10^4 s^{-1} (calc).	Foot..72F028
		For more relative rates see		3.41, 3.60, 3.64.				

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.45	1-chloro-anthracene [R_1 = -Cl]	$CHCl_3$	2.2×10^5	4.5×10^{-2}	rt	Od-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe53F004
3.45.1		CCl_4	4.1×10^5	4.1×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.7×10^3 s^{-1} [*1.8.4*].	Bowe53F004
3.45.2		CS_2	1.0×10^6	4.9×10^{-3}	rt	Od-15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Bowe53F004
3.46	9-chloro-anthracene [R_9 = -Cl]	$CHCl_3$	4.2×10^5	2.4×10^{-2}	rt	Od-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe53F004
3.46.1		CCl_4	5.3×10^5	3.2×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.7×10^3 s^{-1} [*1.8.4*].	Bowe53F004
3.46.2		CS_2	1.7×10^6	3.0×10^{-3}	rt	Od-15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Bowe53F004
3.47	9-methyl-anthracene [R_9 = -Me]	$CHCl_3$	8.3×10^6	1.2×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe53F004
3.47.1		$CHCl_3$	$(8.1 \pm 1.5) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_r^{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
3.47.2		CCl_4	5.2×10^5	3.3×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.7×10^3 s^{-1} [*1.8.4*].	Bowe53F004
3.47.3		C_6H_6	3.2×10^6	$(1.3 \pm 0.3) \times 10^{-2}$	25	A'd-20	S = A' = Rub. k derived using $\beta_{A'}$ = 1.0×10^{-3} mol dm^{-3} [*3.63.18*] and k_d = 4.2×10^4 s^{-1} [*1.32*].	Stev..74F312
3.48	9-methoxy-anthracene [R_9 = -OMe]	C_6H_6	$k_r = 2.5 \times 10^6$		25	Ad-17 A'd	S = A' = Tetr. Measured ($k_r/k_r^{A'}$) = 0.21. k_r derived using $k_r^{A'}$ = *1.2×10^7 dm^3 mol^{-1} s^{-1} [*A3.13*].	Stev..74F312
3.49	1-anthracene-sulfonate ion [R_1 = -SO_3^-]	H_2O	5.0×10^8		28	P'a-23	S = self. Q = NaN_3, A' = KI, P' = I_3^-. k derived using k_d = 5.0×10^5 s^{-1} [*1.1*] and k_Q = 2.2×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*].	Roha.77F074
3.49.1		H_2O	5.4×10^7	9.2×10^{-3}	30	Ad-15	S = self. k derived using k_d = 5.0×10^5 s^{-1} [*1.1*].	Gupt..78A275
3.50	2-anthracene-sulfonate ion [R_2 = -SO_3^-]	H_2O	3.0×10^8		28	P'a-23	S = self. Q = NaN_3, A' = KI, P' = I_3^-. k derived using k_d = 5.0×10^5 s^{-1} [*1.1*] and k_Q = 2.2×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*].	Roha.77F074
3.50.1		H_2O	4.5×10^7	1.1×10^{-2}	30	Ad-15	S = self. k derived using k_d = 5.0×10^5 s^{-1} [*1.1*].	Gupt..78A275
3.51	9-phenyl-anthracene [R_9 = -Ph]	$CHCl_3$	1.4×10^6	7.2×10^{-3}	rt	Od-15	S = self. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Bowe53F004

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.51.1		CCl_4	2.3×10^6	7.4×10^{-4}	rt	Od–15	S = self. k derived using $k_d = *1.7 \times 10^3$ s^{-1} [*1.8.4*].	Bowe53F004
3.51.2		CS_2	6.0×10^6	8.4×10^{-4}	rt	Od–15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Bowe53F004
3.51.3		C_6H_6	4.2×10^5	$(1.0 \pm 0.2) \times 10^{-1}$	25	A'd–20	S = A' = Rub. k derived using $\beta_{A'} = 1.0 \times 10^{-3}$ mol dm^{-3} [*3.63.18*] and $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Stev..74F312
3.52	9,10–dichloro–anthracene [$R_9 = R_{10} = -Cl$]	$CHCl_3$	1.7×10^5	6.0×10^{-2}	rt	Od–15	S = self. k derived using $k_d = *1.0 \times 10^4$ s^{-1} [*1.5.3*].	Bowe53F004
3.52.1		CCl_4	1.7×10^5	1.0×10^{-2}	rt	Od–15	S = self. k derived using $k_d = *1.7 \times 10^3$ s^{-1} [*1.8.4*].	Bowe53F004
3.52.2		CS_2	2.9×10^5	1.7×10^{-2}	rt	Od–15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Bowe53F004
3.53	9,10–dimethyl–anthracene (DMA) [$R_9 = R_{10} = -Me$]	H_2O	9.1×10^8	5.5×10^{-4}	25	Ad–15	S = Eos. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. S and A solubilized in DTAC micelles.	Usui..78F061
3.53.1		H_2O	7.5×10^8	6.6×10^{-4}	25	Ad–15	S = MB. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. A solubilized in DTAC micelles.	Usui..78F061
3.53.2		D_2O	7.4×10^8 $*4.6 \times 10^8$	6.8×10^{-5}	25	Ad–15	S = MB. k derived using $k_d = 5.0 \times 10^4$ ($*3.1 \times 10^4$) s^{-1} [*1.2.3*]. A solubilized in DTAC micelles.	Usui..78F061
3.53.3		MeOH	2.4×10^7 $*1.25 \times 10^7$	$(8.0 \pm 1.5) \times 10^{-3}$	24	Ad–15	S = self. k derived using $k_d = 1.4 \times 10^5$ ($*1.0 \times 10^5$) s^{-1} [*1.3*].	Stev.74F207
3.53.4		MeOH	4.8×10^7 $*3.3 \times 10^7$	$(3.0 \pm 0.6) \times 10^{-3}$	rt	Ad–15	S = MB. k derived using $k_d = 1.4 \times 10^5$ ($*1.0 \times 10^5$) s^{-1} [*1.3*]. Error is a 95% confidence limit.	Beth.77F113
3.53.5		$CHCl_3$	$k_r = 2.7 \times 10^7$ $*1.6 \times 10^7$		24	Ad–17 A'd	S = A' = Rub. Measured $(k_r/k_r^{A'}) = 0.643$. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.14*].	Stev.74F207
3.53.6		$CHCl_3$	9.3×10^7 $*5.6 \times 10^7$	$(1.8 \pm 0.7) \times 10^{-4}$	rt	Ad–15	S = MB. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*]. Error is a 95% confidence limit.	Beth.77F113
3.53.7		CCl_4	$k_r = 7.0 \times 10^6$ $*2.1 \times 10^7$		24	Ad–17 A'd	S = A' = Rub. Measured $(k_r/k_r^{A'}) = 0.5$. k_r derived using $k_r^{A'} = 1.4 \times 10^7$ ($*4.2 \times 10^7$) dm^3 mol^{-1} s^{-1} [*A3.14*].	Stev.74F207

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.53.8	CS_2	$k_r = 1.3 \times 10^7$ *2.1×10^7		24	Ad-17 A'd	S = A' = Rub. Measured ($k_r/k_r^{A'}$) = 0.5. k_r derived using $k_r^{A'} = 2.5 \times 10^7$ (*4.2×10^7) dm^3 mol^{-1} s^{-1} [*A3.14*].	Stev.74F207
3.53.9	CH_3CN	1.7×10^8 *1.3×10^8	$(2.0 \pm 0.4) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*]. Error is a 95% confidence limit.	Beth.77F113
3.53.10	EtOH	1.2×10^7	$(7.2 \pm 1.4) \times 10^{-3}$	24	Ad-15	S = self. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Stev.74F207
3.53.11	EtOH	3.9×10^7	2.1×10^{-3}	25	Ad-15	S = MB. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Usui.78F061
3.53.12	EtOH	4.4×10^7	1.9×10^{-3}	25	Ad-15	S = Eos. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Usui.78F061
3.53.13	CCl_2F-$CClF_2$	4.2×10^5 $k_r = 2.8 \times 10^5$ $k_q = 1.4 \times 10^5$	1.1×10^{-5}	25	Ad-34	$^1O_2$* from Nd-YAG laser (1065 nm). Measured (k_q/k_r) = 0.5. k, k_r, and k_q derived using $k_d = 4.7 \times 10^2$ s^{-1} ([*1(a).2*];[*1(a).2.1*])[a].	Evan.76F417
3.53.14	CCl_2F-$CClF_2$	5.2×10^5 $k_r = 2.9 \times 10^5$ $k_q = 2.2 \times 10^5$	9.1×10^{-5}	25	Ad-34	$^1O_2$* from He/Ne laser (632.8 nm). Measured (k_q/k_r) = 0.76. k, k_r, and k_q derived using $k_d = 4.7 \times 10^2$ s^{-1} ([*1(a).2*];[*1(a).2.1*])[a].	Evan.76F417
3.53.15	C_5H_5N	3.0×10^7		rt	Ad-20	S = MB, A' = TME. Measured ($k_{A'}/k$) = 1.0. k derived using $k_{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Wils66F041
3.53.16	C_5H_5N	4.2×10^7	1.4×10^{-3}	12	Pa-20	S = thionine, A' = TME. k derived using $k_d = 5.9 \times 10^4$ s^{-1} [*1.29.1*].	Kram.73F202
3.53.17	C_5H_5N	5.9×10^7	1.0×10^{-3}	12	Pa-20	S = MB, A' = TME. k derived using $k_d = 5.9 \times 10^4$ s^{-1} [*1.29.1*].	Kram.73F202
3.53.18	C_5H_5N	4.2×10^7	1.4×10^{-3}	12	Pa-20	S = self, A' = TME. k derived using $k_d = 5.9 \times 10^4$ s^{-1} [*1.29.1*].	Kram.73F202
3.53.19	C_6H_{12}	1.2×10^7	$(5.0 \pm 1.0) \times 10^{-3}$	24	Ad-15	S = self. k derived using $k_d = 5.9 \times 10^4$ s^{-1} [*1.30*].	Stev.74F207
3.53.20	C_6H_6	1.3×10^8	3.0×10^{-4}	25	Ad-?	S = Per and anthanthrene. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*]. k is a mean for both S.	Stev.69F388
3.53.21	C_6H_6	1.3×10^8	3.0×10^{-4}	25	Ad-15	S = Rub. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
3.53.22	C_6H_6	1.3×10^8	3.0×10^{-4}	25	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.53.23		C_6H_6	1.3×10^8	3.0×10^{-4}	25	Ad–15	S = Tetr. k derived using $k_d = *4.0 \times 10^4$ s^{-1} [*1.32.9*].	Alga.70E079
3.53.24		C_6H_6	2.1×10^7	$(2.0 \pm 0.5) \times 10^{-3}$	25	Ad–15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Stev..74F312
3.53.25		C_6H_6	3.3×10^7	1.2×10^{-3}	25	Ad–?	S = self. k derived using $k_d = *4.0 \times 10^4$ s^{-1} [*1.32.9*].	Stev..76F422
3.53.26		C_6H_5Br	3.0×10^7		rt	Ad–20	S = MB, A′ = TME. Measured ($k_{A'}/k$) = 1.0. k derived using $k_{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Wils66F041
		For more relative rates see		3.62.5, 3.63.16, 9.1.2, 9.1.4–5, 9.4.2, 9.6.2, 9.6.4, 11.31.4.				
3.54	9,10–dimethoxy–anthracene [$R_9 = R_{10} = -OMe$]	C_6H_6	$k_r = 1.4 \times 10^7$		25	Ad–17 A′d	S = A′ = Rub. Measured ($k_r/k_r^{A'}$) = 0.33. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1}s^{-1} [*3.63.18*].	Stev..74F312
3.55	1,5–anthracene–disulfonate ion [$R_1 = R_5 = -SO_3^-$]	H_2O	$\leqslant 10^7$ (est)		28	P′a–23	S = self, Q = NaN_3, A′ = KI, P′ = I_3^-. No measurable effect.	Roha.77F074
3.55.1		H_2O	7.0×10^6	7.0×10^{-2}	30	Ad–15	S = self. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Gupt..78A275
3.56	9,10–diphenyl–anthracene [$R_9 = R_{10} = -Ph$]	$CHCl_3$	2.5×10^6	4.0×10^{-3}	rt	Od–15	S = self. k derived using $k_d = *1.0 \times 10^4$ s^{-1} [*1.5.3*].	Bowe53F004
3.56.1		$CHCl_3$	$(3.0 \pm 0.4) \times 10^6$		rt	A′d–33	S = A′ = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr78A005
3.56.2		CCl_4	2.8×10^6	6.0×10^{-4}	rt	Od–15	S = self. k derived using $k_d = *1.7 \times 10^3$ s^{-1} [*1.8.4*].	Bowe53F004
3.56.3		CS_2	1.6×10^6	3.2×10^{-3}	rt	Od–15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Bowe53F004
3.56.4		$CFCl_2$–CF_2Cl	$k_r = 4.0 \times 10^5$ (est)		rt	Ad–36	$^1O_2$* directly from CW Nd–YAG laser (1065 nm). Measured ($k_r/k_{O_2}[O_2]$) = 100. k_r estimated using $k_{O_2}[O_2] = 4 \times 10^3$ s^{-1} (based on gas phase value of $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1}).	Math.70F387
3.56.5		C_5H_5N	5.4×10^6		rt	Ad–20	S = self. A′ = TME. Measured ($k_{A'}/k$) = 5.6. k derived using $k_{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Wils66F014
3.56.6		C_6H_6	7.0×10^5	5.7×10^{-2}	rt	Ad–15	S = self. k derived using $k_d = *4.0 \times 10^4$ s^{-1} [*1.32.9*].	Bowe.55F004
3.56.7		C_6H_6	8.9×10^5	4.5×10^{-2}	rt	Ad–15	S = self. k derived using $k_d = *4.0 \times 10^4$ s^{-1} [*1.32.9*].	Livi.59F003

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

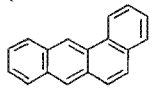
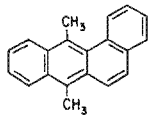
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.56.8		C_6H_6	6.7×10^5	6.0×10^{-2}	rt	Ad-20	S = ZnTPP, A′ = Diphenylanthracene. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Foot.71F580
3.56.9		C_6H_6	1.0×10^6	$(4.0 \pm 0.5) \times 10^{-2}$	25	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev.72F196
3.56.10		C_6H_6	1.2×10^6	$(3.5 \pm 1.0) \times 10^{-2}$	25	A′d-20	S = A′ = Rub. k derived using $\beta_{A'}$ = 1.0×10^{-3} mol dm^{-3} and k_d = 4.2×10^4 s^{-1} [*1.32*].	Stev..74F312
		For more relative rates see		4.28.13, 11.14.3.				
3.57	1-chloro-9,10-diphenylanthracene [R_1 = -Cl, R_9 = R_{10} = -Ph]	$CHCl_3$	$(2.0 \pm 0.5) \times 10^6$		rt	A′d-33	S = A′ = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
3.58	1-methylamino-9,10-diphenylanthracene [R_1 = -NHCH$_3$, R_9 = R_{10} = -Ph]	C_6H_6	3.3×10^8	$(1.2 \pm 0.2) \times 10^{-4}$	25	Ad-15	S = self, A′ = lipoic acid. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.19*].	Stev.75F558
3.59	1,4-dimethoxy-9,10-diphenylanthracene [R_1 = R_4 = -OMe, R_9 = R_{10} = -Ph]	$CHCl_3$	$(3.2 \pm 0.5) \times 10^8$		rt	A′d-33	S = A′ = Rub. k derived using $k_{A'}$ = 5.3×10^7 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr78A005
3.60	1,2-benzanthracene 	C_6H_6	$k_r = 4.8 \times 10^4$		25	Ad-17 A′d	S = A′ = An. Measured $(k_r/k_r^{A'})$ = 0.30. k_r derived using $k_r^{A'}$ = 1.6×10^5 dm^3 mol^{-1} s^{-1} [*3.44.9*].	Stev..74F312
3.61	9,10-dimethyl-1,2-benzanthracene 	H_2O	1.1×10^{10}	4.0×10^{-5}	rt	Ad-15	S = MB. k derived using k_d = *4.4×10^5 s^{-1} [*1.13*]. A solubilized in CTAB micelles.	Gree.78N003
3.61.1		C_6H_6	5.4×10^7	7.4×10^{-4}	25	Ad-?	S = Per and anthanthrene. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*]. k is a mean for both S.	Stev.69F388
3.61.2		C_6H_6	5.6×10^7	7.1×10^{-4}	25	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga..70E079
3.61.3		C_6H_6	5.6×10^7	7.1×10^{-4}	25	Ad-15	S = Tetr. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga..70E079
3.61.4		C_6H_6	4.8×10^7	8.3×10^{-4}	25	Ad-15	S = Rub. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga..70E079
3.61.5		C_6H_6	$k_r = 1.4 \times 10^7$		25	Ad-17 A′d	S = A′ = Rub. Measured $(k_r/k_r^{A'})$ = 0.33. k_r derived using $k_r^{A'}$ = 4.2×10^7 dm^3 mol^{-1} s^{-1} [*3.63.18*].	Stev..74F312

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

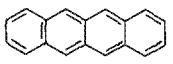
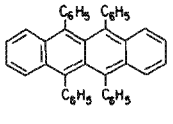
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.61.6		C_6H_6	2.5×10^7	1.6×10^{-3}	25	Ad–?	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev.76F422
		For more relative rates see		3.62.6, 3.63.17.				
3.62	tetracene (2,3–benzanthracene) 	CH_2Cl_2	3.0×10^7	4.0×10^{-4}	rt	Ad–14	S = self. k derived using k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Byst.75F654
3.62.1		CCl_4	$(5.0 \pm 1.5) \times 10^6$		rt	Ld–13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
3.62.2		CCl_4	$k_r = 5 \times 10^6$		rt	Ad–27 28	S = ? k_r derived using $k_A = 5.0 \times 10^6$ dm^3 mol^{-1} s^{-1} [*3.62.1*].	Kras79A010
3.62.3		*n*–BuOH	5.2×10^8	1.0×10^{-4}	20	Ad–15	S = MB. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
3.62.4		C_6H_6	2.4×10^7	1.7×10^{-3}	25	Ad–15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
3.62.5		C_6H_6	$k_r = 8.5 \times 10^6$		25	Pa–17 P'a	S = self. A' = DMA. Measured ($k_r/k_r^{A'}$) = 0.18. k_r derived using $k_r^{A'}$ = *4.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.10*].	Alga.70E079
3.62.6		C_6H_6	$k_r = 1.5 \times 10^7$		25	Pa–17 P'a	S = self, A' = DMBA. Measured ($k_r/k_r^{A'}$) = 0.46. k_r derived using $k_r^{A'}$ = *3.2×10^7 dm^3 mol^{-1} s^{-1} [*A3.12*].	Alga.70E079
3.62.7		C_6H_6	$k_r = 1.2 \times 10^7$		25	Ad–17 A'd	S = A' = rub. Measured ($k_r/k_r^{A'}$) = 0.29. k_r derived using $k_r^{A'}$ = 4.2×10^7 dm^3 mol^{-1} s^{-1} [*3.63.18*].	Stev..74F312
3.62.8		C_6H_6	1.7×10^7	2.4×10^{-3}	25	Ad–?	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev.76F422
		For more relative rates see		3.48, 6.33.3, 7.5.1.				
3.63	5,6,11,12–tetraphenylnaphthacene (Rub) 	MeOH	3.1×10^7 *2.2×10^7	$(4.5 \pm 0.9) \times 10^{-3}$	24	Ad–15	S = self. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^4) s^{-1} [*1.3*].	Stev.74F207
3.63.1		$CHCl_3$	4.25×10^7 *2.5×10^7	$(4.0 \pm 0.8) \times 10^{-4}$	24	Ad–15	S = self. k derived using $k_d = 1.7 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*].	Stev.74F207
3.63.2		$CHCl_3$	5.9×10^7 *3.4×10^7	$(2.9 \pm 1.0) \times 10^{-4}$	25	Ad–15	S = self. k derived using $k_d = 1.7 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*].	Brau.75E223
3.63.3		$CHCl_3$	5.3×10^7 *3.2×10^7	$(3.1 \pm 0.4) \times 10^{-4}$	rt	Ad–15	S = self. k derived using $k_d = 1.7 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*]. k is a mean of 5 measurements.	Monr77F486

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.63.4	CCl_4	1.4×10^7	$(1.0 \pm 0.5) \times 10^{-4}$	24	Ad-15	S = self. k derived using $k_d = 1.4 \times 10^3$ s^{-1} [*1.8*].	Stev.74F207
3.63.5	CCl_4	2.3×10^7	$(6.0 \pm 3.0) \times 10^{-5}$	25	Ad-15	S = self. k derived using $k_d = 1.4 \times 10^3$ s^{-1} [*1.8*].	Brau.75E223
3.63.6	CS_2	2.5×10^7	$(2.0 \pm 0.5) \times 10^{-4}$	24	Ad-15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Stev.74F207
3.63.7	CS_2	5.6×10^7	$(9.0 \pm 3.0) \times 10^{-5}$	25	Ad-15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Brau.75E223
3.63.8	EtOH	2.3×10^7	$(3.6 \pm 0.7) \times 10^{-3}$	24	Ad-15	S = self. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Stev.74F207
3.63.9	$CFCl_2$–CF_2Cl	$k_r = 3.2 \times 10^6$ (est)		rt	Ad-36	$^1O_2$* directly from CW Nd-YAG laser (1065 nm). Measured $(k_r/k_{O_2}[O_2]$ = 800. k_r estimated using $k_{O_2}[O_2] = 4 \times 10^3$ s^{-1} (based on gas phase value of k_{O_2} = 1.3×10^3 dm^3 mol^{-1} s^{-1}).	Math.70F387
3.63.10	C_5H_5N	7.1×10^7		rt	Ad-20	S = MB, A′ = TME. Measured $(k_{A'}/k) = 4.2 \times 10^{-1}$. k derived using $k_{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Wils66F041
3.63.11	C_5H_5N	6.4×10^7		rt	Ad-20	S = self, A′ = TME. Measured $(k_{A'}/k) = 4.7 \times 10^{-1}$. k derived using $k_{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Wils66F041
3.63.12	C_6H_{12}	1.5×10^7	$(4.0 \pm 0.8) \times 10^{-3}$	24	Ad-15	S = self. k derived using $k_d = 5.9 \times 10^4$ s^{-1} [*1.30*].	Stev.74F207
3.63.13	C_6H_6	1.3×10^{10}	3×10^{-6}	rt	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Bowe34F004
3.63.14	C_6H_6	2.4×10^7	1.7×10^{-3}	rt	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Bowe55F004
3.63.15	C_6H_6	1.3×10^8	3.0×10^{-4}	25	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Alga.70E079
3.63.16	C_6H_6	$k_r = 4.7 \times 10^7$		25	Pa-17 P′a	S = self, A′ = DMA. Measured $(k_r/k_r^{A'})$ = 1.0. k_r derived using $k_r^{A'}$ = *4.7×10^7 dm^3 mol^{-1} s^{-1} [*A3.10*].	Alga.70E079
3.63.17	C_6H_6	$k_r = 9.0 \times 10^7$		25	Pa-17 P′a	S = self, A′ = DMBA. Measured $(k_r/k_r^{A'})$ = 2.8. k_r derived using $k_r^{A'}$ = *3.2×10^7 dm^3 mol^{-1} s^{-1} [*A3.12*].	Alga.70E079
3.63.18	C_6H_6	4.2×10^7	$(1.0 \pm 0.1) \times 10^{-3}$	25	Ad-15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Stev..74F312

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

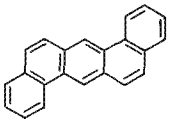
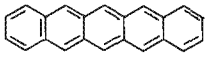
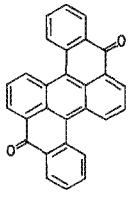
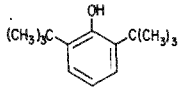
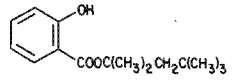
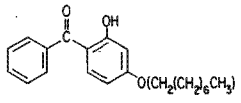
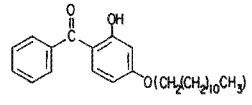
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.63.19		C_6H_6	4.7×10^7	$(8.5 \pm 2.0) \times 10^{-4}$	25	Ad-23	S = self, A′ = lipoic acid. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev..74F641
3.63.20		C_6H_6	$k_r = 4.3 \times 10^7$		25	Ad-17 A′d	S = self, A′ = lipoic acid. Measured $(k_r^{A'}/k_r) = 2.3 \pm 0.5$, k_r derived using $k_r^{A'} = k_{A'} = 1.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*11.45*]. β derived assuming each $^1O_2$* interacting with A′ causes the destruction of 2 molecules of A′.	Stev..74F641
3.63.21		C_6H_6	4.7×10^7	$(9.0 \pm 2.5) \times 10^{-4}$	25	Ad-15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Brau.75E223
3.63.22		C_6H_6	4.0×10^7	1.0×10^{-3}	25	Ad-?	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev.76F422
3.63.23		C_6H_5Br	1.6×10^7	$(8.0 \pm 2.0) \times 10^{-4}$	24	Ad-15	S = self. k derived using $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Stev.74F207
3.63.24		1,2,3-$C_6H_3Cl_3$	5.0×10^7 (est)	$(4.0 \pm 1.5) \times 10^{-4}$	25	Ad-15	S = self. k estimated using $k_d = 2.0 \times 10^4$ s^{-1} (calc).	Brau.75E223
3.63.25		$C_6H_5CH_3$	4.4×10^7	$(9.1 \pm 2.5) \times 10^{-4}$	25	Ad-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.36*].	Brau.75E223
		For more relative rates see		3.53.5, 3.53.7-8, 3.54, 3.61.5, 3.62.7, 5.36.76, 5.36.85, 14.32.11, 14.32.14, 14.34.6.				
3.64	1,2,5,6-dibenz-anthracene 	C_6H_{12}	$k_r = 9.5 \times 10^3$		25	Ad-17 A′d	S = A′ = An. Measured $(k_r/k_r^{A'}) = 0.59$. k_r derived using $k_r^{A'} = 1.6 \times 10^5$ dm^3 mol^{-1} s^{-1} [*3.44.9*].	Stev..74F312
3.65	pentacene 	C_6H_6	$k_r = 4.2 \times 10^9$ *3.4×10^9		25	Ad-17 A′d	S = self, A′ = DPBF. Measured $(k_r/k_r^{A'}) = 6.0$. k_r derived using $k_r^{A'} = 7.0 \times 10^8$ (*6.3×10^8) dm^3 mol^{-1} s^{-1} [*A3.17*].	Stev..74F312
3.66	1,2,7,8-dibenz-perylene-3,9-quinone 	$CHCl_3$	6.8×10^7 *4.0×10^7	$(2.5 \pm 1.0) \times 10^{-4}$	25	Ad-15	S = self. k derived using k_d = 1.7×10^4 (*1.0×10^4) s^{-1} [*1.5*].	Wage.76F570
3.66.1		CCl_4	6.8×10^7	$(2.5 \pm 1.5) \times 10^{-5}$	25	Ad-15	S = self. k derived using $k_d = 1.7 \times 10^3$ s^{-1} [*1.8.4*].	Wage.76F570

TABLE 3. Rate constants for the interaction of singlet oxygen with aromatic hydrocarbons — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
3.66.2		CS_2	8.3×10^7	$(6.0 \pm 1.5) \times 10^{-5}$	25	Ad–15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Wage.76F570
3.66.3		CS_2	8.3×10^7	6.0×10^{-5}	25	Pa–15	S = self. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Drew..77F176
3.66.4		C_6H_6	7.0×10^7	$(6.0 \pm 2.0) \times 10^{-4}$	25	Ad–15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Wage.76F570
3.66.5		C_6H_6	6.7×10^7	6.0×10^{-4}	25	Pa–15	S = self. k derived using k_d = *4.0 $\times 10^4$ s^{-1} [*1.32.9*].	Drew..77F176
3.66.6		$C_6H_5CH_3$	5.8×10^7	$(6.8 \pm 2.0) \times 10^{-4}$	25	Ad–15	S = self. k derived using $k_d = 4.0 \times 10^4$ s^{-1} [*1.36*].	Wage.76F570
3.66.7		1,2,4–$C_6H_3Cl_3$	2.4×10^7 (est)	$(5.5 \pm 1.5) \times 10^{-4}$	25	Ad–15	S = self. k estimated using $k_d(C_6H_5Br) = 1.3 \times 10^4$ s^{-1} [*1.34*].	Wage.76F570

[a]This value of k_d is an average of the k_d values reported under the given entries.

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
4.1	2,6-di-*t*-butyl-phenol 	MeOH	1.01×10^6	1.15×10^{-1}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.1.1		*n*-BuOH	1.7×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.1.2		C_6H_6	3.2×10^4		rt	P'a-20	S = ZnTPP, A' = 2M2P. Measured $(k[A] + k_d)/k_{A'} = 6.17 \times 10^{-2}$ mol dm^{-3} at [A] = 2.2×10^{-1} mol dm^{-3}. k derived using $\beta_{A'} = 5.3 \times 10^{-2}$ mol dm^{-3} [*2.40.23*] and $k_d = 4.17 \times 10^4$ s^{-1} [*1.32*].	Thom.78A171
		For more relative rates see		2.101, 2.101.1.				
4.2	4-(1,1,3,3-tetra-methylbutyl)-phenylsalicylate 	*i*-octane	$\leqslant 1 \times 10^6$ (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.3	2-hydroxy-4-octyloxybenzo-phenone 	C_6H_5Br	$< 1 \times 10^6$ (est)		0	A'd-33	$^1O_2$* from microwave discharge, A' = Rub. No measurable effect.	Guil.73F333
4.3.1		CCl_4 /$CHCl_3$ (9:1) v:v	1.0×10^4 (est)		rt	A'd-23	S = A' = Rub. Measured $k/(k_{A'}[A'] + k_d) = 10.0$ dm^3 mol^{-1} at [A'] = 5×10^{-6} mol dm^{-3}. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
4.4	2-hydroxy-4-dodecyloxybenzo-phenone 	*i*-octane	$< 1 \times 10^6$ (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.4.1		CCl_4 /MeOH (98:2) v:v	$< 2.0 \times 10^5$		rt	A'd-5	S = MB, A' = DPBF, flash photolysis.	Furu.78E238

COMPOUNDS 4.5 - 4.15 :

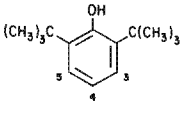


TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.5	4-bromo-2,6-di-*t*-butylphenol [R_4 = -Br]	MeOH	8.41×10^5	1.38×10^{-1}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.5.1		*n*-BuOH	1.5×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Syna...78A266
4.6	4-chloro-2,6-di-*t*-butylphenol [R_4 = -Cl]	*n*-BuOH	3.2×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.7	4-methyl-2,6-di-*t*-butylphenol [R_4 = -Me]	MeOH	5.6×10^6	2.09×10^{-2}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.7.1		MeOH	4.19×10^6	$(2.8 \pm 1.4) \times 10^{-2}$	rt	Pa-15	S = MB. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.7.2		MeOH	$k_r = 2.2 \times 10^5$ *2.9×10^5			Pa-17 P'a	S = MB, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 0.357. k_r derived using $k_r^{A'} = 6.25 \times 10^5$ (*8.1×10^5) dm^3 mol^{-1} s^{-1} [*2.40.2, A3.3*].	Thom.78A171
4.7.3		EtOH	< 1 x 10^9 (est)		0	Od-23	S = MB, A' = DMF. No measurable effect.	Dall..72F518
4.7.4		*n*-BuOH	7.6 x 10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Syna...78A266
4.7.5		C_6H_6	2.53×10^6	1.65×10^{-2}	rt	A'd-16	S = ZnTPP, A' = DPF. k derived using $k_d = 4.17 \times 10^4$ s^{-1} [*1.32*].	Thom.78A171
4.7.6		C_6H_6	8.2×10^5		rt	Pa-20	S = ZnTPP, A' = Car. Measured ($k_{A'}/k_A$) = 1.46 ± 0.11. k derived using $k_{A'} = 1.2 \times 10^{10}$ dm^3 mol^{-1} s^{-1} ([*2.130.12*];[*2.130.14*])[a].	Thom.78A171
4.7.7		C_6H_6	$(6.1 \pm 0.4) \times 10^5$	$(6.5 \pm 1.3) \times 10^{-2}$	rt	Pa-15	S = ZnTPP. k derived using $k_d = 4.17 \times 10^4$ s^{-1} [*1.32*].	Thom.78A171
4.7.8		C_6H_6	6.61×10^5 *7.1×10^5		rt	P'a-20	S = ZnTPP, A' = 2M2P. Measured ($k_A/k_{A'}$) = 8.8×10^{-1}. k derived using $k_{A'} = 7.5 \times 10^5$ (*8.1×10^5) dm^3 mol^{-1} s^{-1} [*2.40.23, A3.3*].	Thom.78A171
4.7.9		C_6H_6	$k_r = 1.2 \times 10^5$ *1.3×10^5		rt	Pa-17 P'a	S = ZnTPP, A' = 2M2P. Measured ($k_r/k_r^{A'}$) = 0.156. k_r derived using $k_r^{A'} = 7.5 \times 10^5$ (*8.1×10^5) dm^3 mol^{-1} s^{-1} [*2.40.23, A3.3*].	Thom.78A171
		For more relative rates see		4.12.				

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.8	4-methoxy-2,6-di-*t*-butylphenol [R_4 = -OCH_3]	*n*-BuOH	2.6×10^7		20	Ad-15	S = MB. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.8.1		*n*-BuOH	2.7×10^7		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.9	4-hydroxy-3,5-di-*t*-butyl benzyl alcohol [R_4 = -CH_2OH]	MeOH	1.47×10^6	7.89×10^{-2}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.9.1		C_6H_6	4.1×10^5 *4.5×10^5		rt	P'a-19	S = ZnTPP, A' = 2M2P. Measured ($k/k_{A'}$) = 0.55. k derived using $k_{A'} = 7.5 \times 10^5$ (*8.1×10^5) dm^3 mol^{-1} s^{-1} [*2.40.23, A3.3*].	Thom.78A171
4.10	4-acetyl-2,6-di-*t*-butylphenol [R_4 = -$COCH_3$]	*n*-BuOH	1.0×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.11	methyl 3,5-di-*t*-butyl-4-hydroxy-benzoate [R_4 = -$COOCH_3$]	*n*-BuOH	9.2×10^5		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.12	2,4,6-tri-*t*-butylphenol [R_6 = -*t*-Bu]	MeOH	3.41×10^6	3.40×10^{-2}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.12.1		MeOH	$k_r = 6.3 \times 10^4$ *8.4×10^4		rt	Pa-17 P'a	S = RB, A' = 2,6-di-*t*-butyl-4-methylphenol. Measured ($k_r/k_r^{A'}$) = 0.29. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*2.9×10^5) dm^3 mol^{-1} s^{-1} [*4.7.2*].	Thom.78A171
4.12.2		*n*-BuOH	3.7×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.12.3		C_6H_6	1.39×10^6	3.0×10^{-2}	rt	A'd-16	S = ZnTPP, A' = DPF. k derived using $k_d = 4.17 \times 10^4$ s^{-1} [*1.32*].	Thom.78A171
4.12.4		C_6H_6	2.56×10^5 *2.8×10^5		rt	P'a-19	S = ZnTPP, A' = 2M2P. Measured ($k_A/k_{A'}$) = 0.34. k derived using $k_{A'} = 7.5 \times 10^5$ (*8.1×10^5) dm^3 mol^{-1} s^{-1} [*2.40.23, A3.3*].	Thom.78A171
4.13	4-*t*-butoxy-2,6-di-*t*-butylphenol [R_4 = -$OC(CH_3)_3$]	*n*-BuOH	2.4×10^7		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Syna...78A266

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

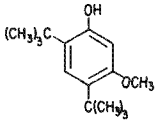
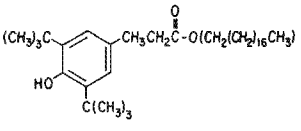
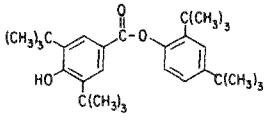
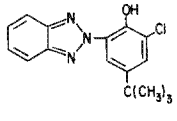
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.14	4-phenyl-2,6-di-*t*-butylphenol [R_4 = -Ph]	MeOH	7.89×10^6	1.47×10^{-2}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.14.1		*n*-BuOH	3.9×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.15	4-benzyl-2,6-di-*t*-butylphenol [R_4 = -$CH_2C_6H_5$]	MeOH	3.76×10^6	3.08×10^{-2}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*][a].	Thom.78A171
4.16	3-methoxy-4,6-di-*t*-butylphenol 	MeOH(?)	$k_r = 2.1 \times 10^5$		rt	Pa-17 P'a	S = RB, A' = TME. Measured ($k_r/k_r^{A'}$) = 7.0×10^{-3}. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Sait..70F454
4.16.1		MeOH(?)	$k_r = 2.0 \times 10^5$		rt	Pa-17 P'a	$^1O_2$* from H_2O_2/NaOCl, A' = TME. Measured ($k_r/k_r^{A'}$) = 6.7×10^{-3}. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Sait..70F454
4.17	octadecyl 3-(3',5'-di-*t*-butyl-4'-hydroxyphenyl) propionate 	*i*-octane	< 1.0×10^6 (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.17.1		CCl_4 /MeOH (98:2) v:v	$(4.6 \pm 0.6) \times 10^5$		rt	A'd-5	S = MB, A' = DPBF, flash photolysis.	Furu.78E238
4.18	2',4'-di-*t*-butylphenyl 3,5-di-*t*-butyl-4-hydroxybenzoate 	C_6H_5Br	⩽ 1.0×10^6 (est)		0	A'd-33	$^1O_2$* from microwave discharge, A' = Rub. No measurable effect.	Guil.73F333
4.18.1		*i*-octane	< 1.0×10^6 (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.19	2-(2'-hydroxy-3'-chloro-5'-*t*-butylphenyl)benzotriazole 	CCl_4 /$CHCl_3$ (9:1) v:v	1.0×10^4 (est)		rt	A'd-23	S = A' = Rub. Measured $k/(k_A[A'] + k_d)$ = 10.0 dm^3 mol^{-1} s^{-1} at [A'] = 5×10^{-6} mol dm^{-3}. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F654

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

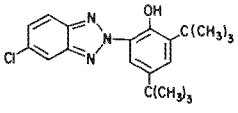
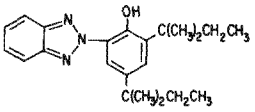
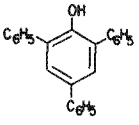
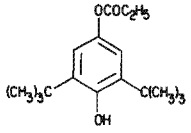
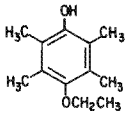
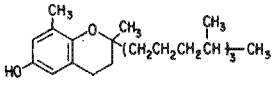
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.20	2-(3',5'-di-*t*-butyl-2'-hydroxyphenyl)-5-chlorobenzotriazole 	C_6H_5Br	2.6×10^6 (est)		0	A'd-33	$^1O_2$* from microwave discharge, A' = Rub. Measured $k/(k_d/[A'] + k_{A'}) = 2.0 \times 10^{-2}$ at $[A'] = 1.5 \times 10^{-4}$ mol dm^{-3}. k estimated using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Guil.73F333
4.21	2-(2'-hydroxy-3',5'-di-*t*-pentylphenyl)benzotriazole 	*i*-octane	$< 1 \times 10^6$ (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.22	2,4,6-triphenylphenol 	MeOH	2.52×10^8	4.6×10^{-4}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.22.1		CH_3CN	1.45×10^7	2.3×10^{-3}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 3.33 \times 10^4$ s^{-1} [*1.17*].	Thom.78A171
4.22.2		C_6H_6	2.2×10^7	1.87×10^{-3}	rt	A'd-16	S = ZnTPP, A' = DPF. k derived using $k_d = 4.17 \times 10^4$ s^{-1} [*1.32*].	Thom.78A171
4.23	3,5-di-*t*-butyl-4-hydroxyphenyl propionate 	MeOH	2.18×10^5	5.34×10^{-1}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.24	durohydroquinone monoethyl ether 	MeOH	7.25×10^7	1.6×10^{-3}	rt	A'd-16	S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5$ s^{-1} ([*1.3*];[*1.3.2*];[*1.3.3*])[a].	Thom.78A171
4.25	δ-tocopherol 	MeOH	7.1×10^7	$(1.4 \pm 0.4) \times 10^{-3}$	25	Ad-15	S = MB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Gram.72A019
4.25.1		EtOH	1.0×10^8	8.3×10^{-4}	20	P'a-22	S = MB, A' = methyllinoleate, P' = methyllinoleate hydroperoxide. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Yama.77F858

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

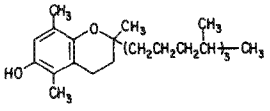
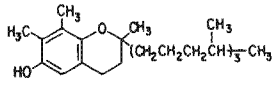
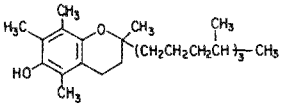
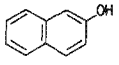
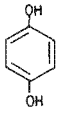
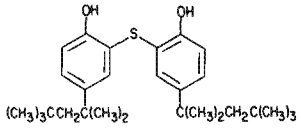
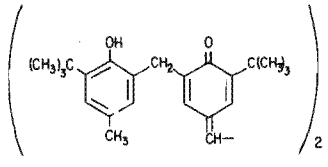
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.25.2		EtOH	$k_r = 2.3 \times 10^6$		20	P'a-17 Ad	S = MB, A' = methyl-linoleate, P' = methyl-linoleate hydroperoxide. Measured ($k_r^{A'}/k_r$) = 9.5×10^{-2}. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ dm^3 mol^{-1} s^{-1} [*14.6*].	Yama.77F858
4.26	β-tocopherol 	MeOH	3.6×10^8	$(2.8 \pm 0.2) \times 10^{-4}$	25	Ad-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Gram.72A019
4.27	γ-tocopherol 	MeOH	1.9×10^8	$(5.4 \pm 0.3) \times 10^{-4}$	25	Ad-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Gram.72A019
4.27.1		EtOH	1.8×10^8	4.5×10^{-4}	20	P'a-22	S = MB, A' = methyl-linoleate, P' = methyl-linoleate hydroperoxide. k derived using k_d = 8.3×10^4 s^{-1} [*1.10*].	Yama.77F858
4.27.2		EtOH	$k_r = 7.9 \times 10^6$		20	P'a-17 Ad	S = MB, A' = methyl-linoleate, P' = methyl-linoleate hydroperoxide. Measured ($k_r^{A'}/k_r$) = 2.8×10^{-2}. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ dm^3 mol^{-1} s^{-1} [*14.6*].	Yama.77F858
4.28	α-tocopherol D_2O 	D_2O	6.4×10^8		rt	A'd-5	S = 2-acetonaphthone, A' = DPBF, N_2 laser (337 nm). A, A', and S solubilized in SDS micelles.	Gorm.78E144
4.28.1		MeOH	7.1×10^8	$(1.4 \pm 0.4) \times 10^{-4}$	25	Ad-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Gram.72A019
4.28.2		MeOH	$(6.7 \pm 0.6) \times 10^8$ *4.8×10^8	$(2.1 \pm 0.2) \times 10^{-4}$	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*].	Foot..74R113
4.28.3		MeOH	$k_r = (4.6 \pm 1.0) \times 10^7$ *2.0×10^7		rt	Ad-17 A'd	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 0.29. k_r derived using $k_r^{A'} = 1.56 \times 10^8$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Foot..74R113
4.28.4		CCl_4	$(1.0 \pm 0.3) \times 10^8$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.28.5		EtOH	2.6×10^8	3.2×10^{-4}	20	P'a-22	S = MB, A' = methyl linoleate, P' = methyl linoleate hydroperoxide. k derived using k_d = 8.3×10^4 s^{-1} [*1.10*].	Yama.77F858
4.28.6		EtOH	$k_r = 2.0 \times 10^7$		20	P'a-17 Ad	S = MB, A' = methyl linoleate, P' = methyl linoleate hydroperoxide. Measured ($k_r/k_r^{A'}$) = 1.1×10^{-2}. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ dm^3 mol^{-1} s^{-1} [*14.6*].	Yama.77F858
4.28.7		EtOH	1.05×10^8 (est)		rt	A'd-19	S = RB, A' = chloro-phyll-a. k derived using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
4.28.8		CCl_2F-$CClF_2$	$(3.1 \pm 1.2) \times 10^7$		rt	A'd-23	$^1O_2$* from Nd-YAG (CW) laser (1065 nm), A' = bilirubin. k derived using $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value [74F102]).	Brab.76F425
4.28.9		CCl_2F-$CClF_2$	$k_r = (1.9 \pm 0.5) \times 10^6$		rt	Ad-36	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using k_{O_2} = 2.7×10^3 dm^3 mol^{-1} s^{-1} (gas phase value [74F102]).	Brab.76F425
4.28.10		C_5H_5N	$(2.5 \pm 0.1) \times 10^8$		rt	A'd-23	S = A' = Rub. k derived using $k_{A'}$ = 4×10^7 dm^3 mol^{-1} s^{-1} [74F207] and k_d = *6.0×10^4 s^{-1} [*1.29.1*].	Fahr...74R112
4.28.11		C_5H_5N	$k_r = 1.2 \times 10^6$		rt	Ad-14 28	S = protoporphyrin, A' = chorophyll-a. k_r derived using $\beta_{A'} = 0.9$ mol dm^{-3}, $k_A = 2.5 \times 10^8$ dm^3 mol^{-1} s^{-1} [*4.28.10*] and k_d = *6.0×10^4 s^{-1} [*1.29.1*].	Fahr...74R112
4.28.12		C_6H_{12}	9.0×10^7	$(6.8 \pm 0.8) \times 10^{-4}$	25	A'd-23	S = A' = Rub. k derived using $\beta_{A'}$ = 1.4×10^{-3} dm^3 mol^{-1} s^{-1} [74F207] and $k_d = 5.9 \times 10^4$ s^{-1} [*1.30*].	Stev..74R114
4.28.13		C_6H_{12}	$k_r = 1.1 \times 10^6$ *1.4×10^6		25	Ad-17 A'd	S = A' = 9,10-diphenyl-anthracene. Measured ($k_r/k_r^{A'}$) = 0.9 ± 0.1. k_r derived using $k_r^{A'}$ = 1.2×10^6 (*1.5×10^6) dm^3 mol^{-1} s^{-1} [*3.56.10, A3.11*].	Stev..74R114
4.28.14		C_6H_6	1.7×10^8	$(2.7 \pm 0.4) \times 10^{-4}$	25	A'd-23	S = A' = Rub. k derived using $\beta_{A'}$ = 1.0×10^{-3} dm^3 mol^{-1} s^{-1} [*3.63.18*] and $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Stev..74R114

TABLE 4. Rate constants for the interaction of singlet oxygen with phenols and naphthols — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
4.28.15		*i*-octane	$(1.2 \pm 0.1) \times 10^8$		rt	A'd-23	S = A' = Rub. k derived using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} [74F207] and k_d (unreported).	Fahr...74R112
4.29	α-naphthol 	*n*-BuOH	3.2×10^7		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.30	β-naphthol 	*n*-BuOH	7.6×10^6		20	A'd-23	S = MB, A' = Tetr. k derived using $k_{A'} = 5.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*3.62.3*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Snya...78A266
4.31	hydroquinone 	C_5H_5N	6.9×10^7		rt	A'd-23	S = A' = Rub. k derived using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} [74F207] and $k_d = {}^*6.0 \times 10^4$ s^{-1} [*1.29.1*].	Fahr...74R112
4.31.1		C_6H_6 /MeOH (4:1) v:v	7.0×10^7 ${}^*2.7 \times 10^7$		25	P'a-20	S = MB, A' = 2M2P. k derived using $\beta_{A'} = 4 \times 10^{-2}$ mol dm^{-3} and $k_d = 1.0 \times 10^5$ (${}^*3.8 \times 10^4$) s^{-1} [*1.49*].	Foot....70F734
4.31.2		EtOH/H_2O (95:5) v:v	$(5.8 \pm 2.4) \times 10^8$		rt	Ld-13	$^1O_2$* from pyrogallol autooxidation by O_2/KOH. k measured by monitoring the quenching of chemiluminescence by A.	Slaw78F605
4.32	2,2'-thiobis[4-(1,1,3,3-tetramethylbutyl)phenol] 	*i*-octane	$< 1.0 \times 10^6$ (est)		rt	A'd-23	S = A' = Rub. No measurable effect.	Carl..73P066
4.33		CH_2Cl_2	8.2×10^9		30	Od-23	S = MB, A' = TME. k derived using $k_{A'} = {}^*3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*] and $k_d = {}^*1.2 \times 10^4$ s^{-1} [*1.4.2*].	Taim.76F921

*This value of k_d is an average of the k_d values reported under the given entries.

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
			COMPOUNDS 5.1 - 5.33 :					
								
5.1	furan	MeOH	2.2×10^7	4.5×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 0.84 kJ mol^{-1}.	Koch68F288
5.1.1		MeOH	3.8×10^7	2.6×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.2	2-methylfuran [R_2 = -Me]	H_2O (pH 7.0)	1.0×10^8		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in Triton X-100 micelles (1% by volume).	Barb.78A278
5.2.1		H_2O (pH 7.0)	1.1×10^8		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in Triton X-100 micelles (2% by volume).	Barb.78A278
5.2.2		H_2O (pH 7.0)	1.0×10^8		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in Triton X-100 micelles (5% by volume).	Barb.78A278
5.2.3		H_2O (pH 7.0)	7.0×10^7		rt	Od-19	S = hematoporphyrin Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in Triton X-100 micelles (1% by volume).	Barb.78A278
5.2.4		H_2O (pH 7.0)	6.0×10^7		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Barb.78A278
5.2.5		MeOH	2.6×10^7	3.8×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 1.7 kJ mol^{-1}.	Koch68F288
5.2.6		MeOH	9.1×10^7	$(1.1 \pm 0.2) \times 10^{-3}$	23	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn..71F398
5.2.7		MeOH	9.1×10^7	1.1×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.2.8		n-BuOH	4.3×10^7	$(1.2 \pm 0.2) \times 10^{-3}$	23	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Youn..71F398
5.2.9		t-BuOH	4.3×10^7	$(6.9 \pm 0.7) \times 10^{-4}$	23	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Youn..71F398
5.3	furfurylamine [R_2 = -CH_2NH_2]	MeOH	1.1×10^7	9.0×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 2.9 kJ mol^{-1}.	Koch68F288
5.3.1		MeOH	3.3×10^6	3.0×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.4	furfural [R_2 = -CHO]	MeOH	1.7×10^5	6.0×10^{-1}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 21 kJ mol^{-1}.	Koch68F288
5.4.1		MeOH	1.25×10^6	8.0×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.5	2-methoxyfuran [R_2 = -OMe]	MeOH	2.5×10^8	4.0×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.6	furfuryl alcohol [R_2 = -CH_2OH]	H_2O	2.4×10^8	1.8×10^{-3}	rt	Od-14	S = proflavin. k derived using $k_d = *4.4 \times 10^5$ s^{-1} [*1.1.3*].	Sluy61F008
5.6.1		MeOH	3.0×10^7	3.3×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 2.9 kJ mol^{-1}.	Koch68F288
5.6.2		MeOH	2.1×10^7	4.7×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.7	furfuryl-methylether	MeOH	2.9×10^7	3.4×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 5.0 kJ mol^{-1}.	Koch68F288
5.8	2-furoic acid [R_2 = -COOH]	MeOH	8.3×10^6	1.2×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.9	2-vinylfuran [R_2 = -CH=CH_2]	MeOH	5.6×10^7	1.8×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 3.8 kJ mol^{-1}.	Koch68F288
5.10	α-methylfurfuryl alcohol [R_2 = -CH(OH)CH_3]	MeOH	1.04×10^8	8.73×10^{-4}	25	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 9.0 \times 10^4$ s^{-1} ([*1.3.2*];[*1.3.3*]).[b]	Mart72F519
5.11	α-phenylfurfuryl alcohol [R_2 = -CH(OH)C_6H_5]	MeOH	5.15×10^6	1.77×10^{-2}	25	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 9.0 \times 10^4$ s^{-1} ([*1.3.2*];[*1.3.3*].[b]	Mart72F519

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.12	α-benzylfurfuryl alcohol [R_2 = -CH(OH)$CH_2C_6H_5$]	MeOH	1.09×10^7	8.35×10^{-3}	25	A'd-16	S = RB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3].[b]	Mart72F519
5.13	α-phenethyl-furfuryl alcohol [R_2 = -CH(OH)$(CH_2)_2C_6H_5$]	MeOH	2.54×10^7	3.58×10^{-3}	25	A'd-16	S = RB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3].[b]	Mart72F519
5.14	α-(3-phenylpropyl)-furfuryl alcohol [R_2 = - CH(OH)$(CH_2)_3C_6H_5$]	MeOH	8.94×10^8	1.02×10^{-4}	25	A'd-16	S = RB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3].[b]	Mart72F519
5.15	α-benzhydryl-furfuryl alcohol [R_2 = -CH(OH)$CH(C_6H_5)_2$]	MeOH	1.14×10^7	8.0×10^{-3}	25	A'd-16	S = RB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3].[b]	Mart72F519
5.16	α,α-diphenylfur-furyl alcohol [R_2 = -C(OH)$(C_6H_5)_2$]	MeOH	9.9×10^6	9.2×10^{-3}	25	A'd-16	S = RB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3].[b]	Mart72F519
5.17	2-acetylfuran [R_2 = -$COCH_3$]	MeOH	4.5×10^6	2.2×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [1.3.6].	Youn....72F510
5.18	*N*-methylfurfuryl-amine [R_2 = -$CH_2NH(CH_3)$]	MeOH	7.7×10^6	1.3×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [1.3.6]. E_a = 4.2 kJ mol^{-1}.	Koch68F288
5.19	2-phenylfuran [R_2 = -Ph]	MeOH	$k_r = 3.9 \times 10^7$		25	Ad-17 A'd	S = RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 0.558. k_r derived using $k_r^{A'}$ = *7.0×10^7 dm^3 mol^{-1} s^{-1} [A3.16].	Youn..71F398
5.19.1		MeOH	$k_r = 3.9 \times 10^7$		rt	Ad-17 A'd	S=MB or RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 0.558. k_r derived using $k_r^{A'}$ = *7.0×10^7 dm^3 mol^{-1} s^{-1} [A3.16].	Youn....72F510
5.19.2		*n*-BuOH	$k_r = 2.6 \times 10^7$ *1.8×10^7	β_r = 2.0×10^{-3} *2.9×10^{-3}	25	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 2.1. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [5.30.5] and k_d = 5.2×10^4 s^{-1} [1.24].	Youn..71F398
5.19.3		*t*-BuOH	$k_r = 8.8 \times 10^6$ *6.0×10^6	β_r = 3.4×10^{-3} *5.0×10^{-3}	25	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 3.58. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [5.30.5] and k_d = 3.0×10^4 s^{-1} [1.25].	Youn..71F398
5.20	3-phenylfuran [R_3 = -Ph]	MeOH	3.6×10^7	2.8×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [1.3.6].	Youn....72F510
5.21	3-(4'-fluoro-phenyl)furan [R_3 = 4'-FC_6H_4-]	MeOH	2.9×10^7	3.4×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [1.3.6].	Youn....72F510

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.22	2-(4′-chloro-phenyl)furan [R_2 = 4′-ClC_6H_4-]	MeOH	$k_r = 2.5 \times 10^7$		25	Ad-17 A′d	S = RB , A′ = DPF. Measured ($k_r/k_r^{A'}$) = 0.352. k_r derived using $k_r^{A'}$ = *7.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.16*].	Youn..71F398
5.22.1		MeOH	3.4 × 10^7	2.9 × 10^{-3}	rt	A′d-16	S = MB, A′ = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn....72F510
5.22.2		*n*-BuOH	k_r = 1.5 × 10^7 *1.0 × 10^7	β_r = 3.4 × 10^{-3} *5.0 × 10^{-3}	25	Ad-17 A′d (sep)	S = RB, A′ = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 3.58. k_r derived using $\beta_r^{A'}$ = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 5.2 × 10^4 s^{-1} [*1.24*].	Youn..71F398
5.22.3		*t*-BuOH	k_r = 8.6 × 10^5 *5.8 × 10^5	β_r = 3.5 × 10^{-2} *5.2 × 10^{-2}	25	Ad-17 A′d (sep)	S = RB, A′ = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 36.8. k_r derived using $\beta_r^{A'}$ = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 3.0 × 10^4 s^{-1} [*1.24*].	Youn..71F398
5.23	3-(4′-bromo-phenyl)furan [R_3 = 4′-BrC_6H_4-]	MeOH	2.3 × 10^7	4.4 × 10^{-3}	rt	A′d-16	S = MB, A′ = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn....72F510
5.24	2-(4′-methyl-phenyl)furan [R_2 = 4′-$CH_3C_6H_4$-]	MeOH	k_r = 4.8 × 10^7		rt	Ad-17 A′d	S=MB or RB, A′ = DPF. Measured ($k_r/k_r^{A'}$) = 0.679. k_r derived using $k_r^{A'}$ = *7.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.16*].	Youn....72F510
5.25	3-(4′-methyl-phenyl)furan [R_3 = 4′-$CH_3C_6H_4$-]	MeOH	4.2 × 10^7	2.4 × 10^{-3}	rt	A′d-16	S=RB or MB, A′ = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn....72F510
5.26	2-(4′-methoxy-phenyl)furan [R_2 = 4′-$MeOC_6H_4$-]	H_2O	k_r = 7.5 × 10^8 *5.1 × 10^8	β_r = 5.9 × 10^{-4} *8.7 × 10^{-4}	rt	Ad-17 A′d (sep)	S=MB or RB, A′ = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 0.618. k_r derived using $\beta_r^{A'}$ = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = *4.4 × 10^5 s^{-1} [*1.1.3*].	Youn....72F510
5.26.1		MeOH	k_r = 6.4 × 10^7		rt	Ad-17 A′d	S=MB or RB, A′ = DPF. Measured ($k_r/k_r^{A'}$) = 0.92. k_r derived using $k_r^{A'}$ = *7.0 × 10^7 dm^3 mol^{-1} s^{-1} [*A3.16*].	Youn....72F510
5.26.2		glycol	k_r = 4.7 × 10^8 *3.2 × 10^8	β_r = 3.4 × 10^{-4} *5.0 × 10^{-4}	rt	Ad-17 A′d (sep)	S=MB or RB, A′ = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 0.36. k_r derived using $\beta_r^{A'}$ = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = *1.6 × 10^5 s^{-1} [*1.11.1*].	Youn....72F510
5.26.3		*n*-BuOH	k_r = 2.7 × 10^7 *1.9 × 10^7	β_r = 1.9 × 10^{-3} *2.8 × 10^{-3}	rt	Ad-17 A′d (sep)	S=RB or MB, A′ = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 2.0. k_r derived using $\beta_r^{A'}$ = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 5.2 × 10^4 s^{-1} [*1.24*].	Youn....72F510

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.27	3-(4'-methoxy-phenyl)furan [R_3 = 4'-$MeOC_6H_4$-]	MeOH	5.3×10^7	1.9×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.28	2,4-dimethylfuran [R_2 = R_4 = -Me]	MeOH	5.0×10^7	2.0×10^{-3}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 6.3 kJ mol^{-1}.	Koch68F288
5.29	2,5-dimethylfuran [R_2 = R_5 = -Me]	H_2O	1.7×10^9 $*1.5 \times 10^9$	$(3.0 \pm 0.6) \times 10^{-4}$	25	Ad-15	S = MB. k derived using $k_d = 5.0 \times 10^5$ ($*4.4 \times 10^5$) s^{-1} [*1.1*].	Usui.74F044
5.29.1		H_2O	1.56×10^9	3.2×10^{-4}	25	Ad-15	S = MB. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Usui..78F061
5.29.2		H_2O	1.5×10^9 $*1.4 \times 10^9$	$(3.2 \pm 0.6) \times 10^{-4}$	25	Ad-15	S = MB. k derived using $k_d = 5.0 \times 10^5$ ($*4.4 \times 10^5$) s^{-1} [*1.1*].	Usui.74F044
5.29.2a		H_2O	8.0×10^8	5.5×10^{-4}	25	Od-15	$^1O_2$* from H_2O_2/NaOCl. k derived using $k_d = *4.4 \times 10^5$ s^{-1} [*1.1.3*].	Held...78A227
5.29.3		MeOH	$\sim 5.0 \times 10^8$	$\sim 2.0 \times 10^{-4}$	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 4.2 kJ mol^{-1}.	Koch68F288
5.29.4		MeOH	3.6×10^8	$(2.8 \pm 0.3) \times 10^{-4}$	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn..71F398
5.29.5		MeOH	$(4.0 \pm 1.0) \times 10^8$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Merk.72F260
5.29.6		MeOH	3.6×10^8	2.8×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....72F510
5.29.7		MeOH	1.0×10^8	1.0×10^{-3}	rt	Od-?	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.75F652
5.29.8		MeOH	3.9×10^8	2.8×10^{-4}	25	Ad-15	S = MB. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.5*].	Usui..78F061
5.29.9		EtOH	2.4×10^7	3.28×10^{-3}	0	Od-20	S = MB, A' = 1-cyclo-hexylamino-4-phenyl-amino benzene. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*].	Dall..72F518
5.29.10		EtOH	3.8×10^8	2.2×10^{-4}	25	Ad-15	S = MB. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Usui..78F061
5.29.11		EtOH	4.9×10^8	1.6×10^{-4}	rt	Ad-15	S = retinal. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*].	Delm.78F201
5.29.12		EtOH	5.3×10^8	1.5×10^{-4}	rt	Ad-15	S = MB. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*].	Delm.78F201

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.29.13		$CFCl_2$–CF_2Cl	8.0×10^6 (est)		rt	A′d–37	$^1O_2$* from Nd–YAG CW laser (1065 nm), A′ = Rub. Measured $k/k_{O_2}[O_2] = 2 \times 10^3$ dm^3 mol^{-1}. k estimated using $k_{O_2}[O_2] = 4 \times 10^3$ s^{-1} (based on gas phase value of $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1}).	Math.70F387
5.29.14		$(Me)_2CO$	2.1×10^8 *1.7×10^8	1.8×10^{-4}	rt	Od–?	S = MB. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Ligh.75F652
5.29.15		MeOH /*t*-BuOH (1:1) v:v	$k_r = 7.2 \times 10^7$		rt	Ad–17 A′d	S = RB, A′ = TME. Measured $(k_r/k_r^{A'}) = 2.4$. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
5.29.16		MeOH /*t*-BuOH (1:1) v:v	$k_r = 1.6 \times 10^8$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/NaOCl, A′ = TME. Measured $(k_r/k_r^{A'}) = 5.2$. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
5.29.17		MeOH /*t*-BuOH (1:1) v:v	$k_r = 4.5 \times 10^7$		rt	Ad–17 A′d	$^1O_2$* from H_2O_2/$Ca(OCl)_2$, A′ = TME. Measured $(k_r/k_r^{A'}) = 1.5$. k_r derived using $k_r^{A'}$ = *3.0×10^7 dm^3 mol^{-1} s^{-1} [*A3.2*].	Higg..68F292
5.29.18		MeOH /*t*-BuOH (1:1) v:v	4.9×10^8 (est)	$(1.6 \pm 0.2) \times 10^{-4}$	rt	A′d–16	S = RB, A′ = DPBF. k estimated using $k_d = 7.9 \times 10^4$ s^{-1} (calc).	Youn..71F398
		For more relative rates see		7.17, 7.17.1.				
5.30	2,5-diphenylfuran [$R_2 = R_5 = -Ph$]	H_2O	$k_r = 9.6 \times 10^8$ *6.5×10^8	$\beta_r = 4.58 \times 10^{-4}$ *6.7×10^{-4}	rt	Ad–17 A′d (sep)	S = RB. Measured $(\beta_r/\beta_r(MeOH)) = 0.481$. k_r derived using $\beta_r(MeOH) = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = *4.4×10^5 s^{-1} [*1.1.3*].	Youn..71F398
5.30.1		D_2O	$k_r = 4.0 \times 10^8$	$\beta_r = 7.7 \times 10^{-5}$	23	Ad–17 A′d (sep)	S = MB. Measured $(\beta_r/\beta_r(H_2O)) = 0.115$. k_r derived using $\beta_r(H_2O) = 6.7 \times 10^{-4}$ mol dm^{-3} [*5.30*] and k_d = *3.1×10^4 s^{-1} [*1.2.3*].	Port.74R214
5.30.2		D_2O (pD 7.1)	$k_r = 2.5 \times 10^8$	$\beta_r = 1.2 \times 10^{-4}$	23	Ad–17 A′d (sep)	S = MB. Measured $(\beta_r/\beta_r(H_2O)) = 0.182$. k_r derived using $\beta_r(H_2O) = 6.7 \times 10^{-4}$ mol dm^{-3} [*5.30*] and k_d = *3.1×10^4 s^{-1} [*1.2.3*].	Port.74R214
5.30.3		D_2O (pD 7.1)	$k_r = 2.2 \times 10^8$	$\beta_r = 1.4 \times 10^{-4}$	23	Ad–17 A′d (sep)	S = MB. Measured $(\beta_r/\beta_r(H_2O)) = 0.206$. k_r derived using $\beta_r(H_2O) = 6.7 \times 10^{-4}$ mol dm^{-3} [*5.30*] and k_d = *3.1×10^4 s^{-1} [*1.2.3*]. solvent contains 960 μM H_2O_2.	Port.74R214

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.30.4		D_2O (pD 7.1)	$k_r = 2.8 \times 10^8$	$\beta_r = 1.1 \times 10^{-4}$	23	Ad–17 A'd (sep)	S = MB. Measured $(\beta_r/\beta_r(H_2O)) = 0.165$. k_r derived using $\beta_r(H_2O) = 6.7 \times 10^{-4}$ mol dm^{-3} [*5.30*] and k_d = *3.1 × 10^4 s^{-1} [*1.2.3*]. 1 μl/ml of catalase present in reaction medium.	Port.74R214
5.30.5		MeOH	1.1×10^8	$(9.5 \pm 1.0) \times 10^{-4}$	25	A'd–16	S = RB, A' = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn..71F398
5.30.6		MeOH	$(4.6 \pm 0.8) \times 10^7$		rt	A'd–8	S = RB, A' = DPBF, dye laser (583 nm).[a]	Youn..73F014
5.30.7		MeOH	$k_r \approx 5 \times 10^5$ *3.6 × 10^5		rt	Ad–14	S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10^5) s^{-1} [*1.3*] and $\phi_{isc} = 0.76$.	Olms.73F660
5.30.8		MeOH	1.1×10^8	8.82×10^{-4}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Brew74F646
5.30.9		CH_2Cl_2	8.6×10^7	1.39×10^{-4}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *1.2 × 10^4 s^{-1} [*1.4.2*].	Brew74F646
5.30.10		$CHCl_3$	4.9×10^7	2.04×10^{-4}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *1.0 × 10^4 s^{-1} [*1.5.3*].	Brew74F646
5.30.11		glycol	$k_r = 4.6 \times 10^8$ *3.1 × 10^8	$\beta_r = 3.5 \times 10^{-4}$ *5.1 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured $(\beta_r/\beta_r(MeOH)) = 0.366$. k_r derived using $\beta_r(MeOH) = 9.5 \times 10^{-4}$ (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 1.6 × 10^5 s^{-1} [*1.11.1*].	Youn..71F398
5.30.12		CH_3CN	2.0×10^8	1.3×10^{-4}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *2.55 × 10^4 s^{-1} [*1.17.2*].	Brew74F646
5.30.13		*i*-PrOH	4.8×10^7	1.04×10^{-3}	rt	A'd–16	S = MB, A' = DPBF. k derived using $k_d = 5.0 \times 10^4$ s^{-1} [*1.19*]. Solvent contained 1% MeOH.	Brew74F646
5.30.14		$(Me)_2CO$	1.8×10^8	1.7×10^{-4}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *3.1 × 10^4 s^{-1} [*1.22.2*].	Brew74F646
5.30.15		*n*-BuOH	$k_r = 5.3 \times 10^7$ *3.6 × 10^7	$\beta_r = 9.8 \times 10^{-4}$ *1.4 × 10^{-3}	25	Ad–17 A'd (sep)	S = RB. Measured $(\beta_r/\beta_r(MeOH)) = 1.03$. k_r derived using $\beta_r(MeOH) = 9.5 \times 10^{-4}$ (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 5.2 × 10^4 s^{-1} [*1.24*].	Youn.71F398

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.30.16		n-BuOH	5.0×10^7	1.04×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*]. Solvent contained 1% MeOH.	Brew74F646
5.30.17		t-BuOH	$k_r = 3.75 \times 10^7$ *2.5×10^7	$\beta_r =$ 8.0×10^{-4} *1.2×10^{-3}	25	Ad-17 A'd (sep)	S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.842$. k_r derived using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and $k_d =$ 3.0×10^4 s^{-1} [*1.25*].	Youn.71F398
5.30.18		t-BuOH	3.6×10^7	8.3×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*]. Solvent contained 1% MeOH.	Brew74F646
5.30.19		ethyl acetate	3.0×10^7	6.9×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 2.1 \times 10^4$ s^{-1} [*1.28*].	Brew74F646
5.30.20		dioxane	2.7×10^7	1.07×10^{-3}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 2.9 \times 10^4$ s^{-1} [*1.27*].	Brew74F646
5.30.21		THF	7.5×10^7	5.9×10^{-4}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 4.3 \times 10^4$ s^{-1} [*1.26*].	Brew74F646
5.30.22		C_5H_5N	6.1×10^7	9.9×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d =$ *6.0×10^4 s^{-1} [*1.29.1*]. Solvent contained 1% MeOH.	Brew74F646
5.30.23		$C_6H_{11}OH$	5.3×10^7	1.17×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 6.2 \times 10^4$ s^{-1} [*1.31*]. Solvent contained 1% MeOH.	Brew74F646
5.30.24		methyl benzoate	4.12×10^7	6.07×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = 2.5 \times 10^4$ s^{-1} [*1.37*]. Solvent contained 1% MeOH.	Brew74F646
5.30.25		MeOH/H_2O (81:19) Mole %	$k_r = 2.9 \times 10^8$ *1.9×10^8 (est)	$\beta_r =$ 7.7×10^{-4} *1.1×10^{-3}	rt	Ad-17 A'd (sep)	S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.806$. k_r estimated using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and $k_d =$ 2.2×10^5 s^{-1} (calc).	Youn..71F398
5.30.26		MeOH/H_2O (66:34) Mole %	$k_r = 4.7 \times 10^8$ *3.2×10^8 (est)	$\beta_r =$ 5.9×10^{-4} *8.7×10^{-4}	rt	Ad-17 A'd (sep)	S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.621$. k_r estimated using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and $k_d =$ 2.8×10^5 s^{-1} (calc).	Youn..71F398

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

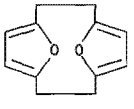
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.30.27		MeOH/H_2O (40:60) Mole %	$k_r = 8.5\times10^8$ *5.8 × 10^8 (est)	β_r = 4.2 × 10^{-4} *6.2 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured (β_r/β_r(MeOH)) = 0.446. k_r estimated using β_r(MeOH) = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 3.6 × 10^5 s^{-1} (calc).	Youn..71F398
5.30.28		MeOH/H_2O (12:88) Mole %	$k_r = 1.0\times10^9$ *6.8 × 10^8 (est)	β_r = 4.2 × 10^{-4} *6.1 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured (β_r/β_r(MeOH)) = 0.439. k_r estimated using β_r(MeOH) = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 4.2 × 10^5 s^{-1} (calc).	Youn..71F398
5.30.29		MeOH /glycol (3:1) v:v	2.0 × 10^8 *1.4 × 10^8 (est)	β_r = 5.5 × 10^{-4} *8.1 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured (β_r/β_r(MeOH)) = 0.578. k_r derived using β_r(MeOH) = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 1.1 × 10^5 s^{-1} (calc).	Youn..71F398
5.30.30		MeOH /glycol (1:1) v:v	3.8 × 10^8 *2.6 × 10^8 (est)	β_r = 3.4 × 10^{-4} *5.0 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured (β_r/β_r(MeOH)) = 0.355. k_r derived using β_r(MeOH) = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 1.3 × 10^5 s^{-1} (calc.).	Youn..71F398
5.30.31		MeOH /glycol (1:3) v:v	5.4 × 10^8 *3.6 × 10^8 (est)	β_r = 2.6 × 10^{-4} *3.9 × 10^{-4}	rt	Ad–17 A'd (sep)	S = RB. Measured (β_r/β_r(MeOH)) = 0.278. k_r derived using β_r(MeOH) = 9.5 × 10^{-4} (*1.4 × 10^{-3}) mol dm^{-3} [*5.30.5*] and k_d = 1.4 × 10^5 s^{-1} (calc).	Youn..71F398
		For more relative rates see	4.28.3, 5.19, 5.19.1–3, 5.22, 5.22.2–3, 5.24, 5.26, 5.26.1–3, 5.36.7, 5.36.13, 5.36.21, 5.36.25, 5.36.42, 5.36.45, 5.36.55, 5.36.58, 5.36.61, 5.36.64–5, 5.36.68–9, 5.36.72, 5.36.74, 5.36.78, 5.36.82, 5.36.113.					
5.31	3,4–diphenylfuran [$R_3 = R_4 =$ –Ph]	MeOH	6.0 × 10^7	1.67 × 10^{-3}	rt	A'd–16	S=RB or MB, A' = DPBF. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Youn....72F510
5.32	3,4–diethoxy–carbonylfuran [$R_3 = R_4 =$ –$COOC_2H_5$]	MeOH	≈ 5.0 × 10^5	≈ 2.0 × 10^{-1}	20	Od–15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 12.6 kJ mol^{-1}.	Koch68F288
5.33	2,3,4,5–tetra–phenylfuran [$R_2 = R_3 = R_4 = R_5$ = –Ph]	MeOH	≈ 3.3 × 10^6	≈ 3.0 × 10^{-2}	20	Od–15	S = RB. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*]. E_a = 4.2 kJ mol^{-1}.	Koch68F288
5.34	2,2(2,5)furan–ophane 	MeOH	1.6 × 10^8	5.47 × 10^{-4}	25	A'd–16	S = RB, A' = DPBF. k derived using k_d = 9.0 × 10^4 s^{-1} ([*1.3.2*];[*1.3.3*]).[b]	Mart72F519

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

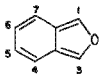
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
			COMPOUNDS 5.35 - 5.39 : 					
5.35	isobenzofuran	MeOH	9.2×10^7	9.83×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = 9.0×10^4 s^{-1} ([1.3.2];[1.3.3]).[b]	Youn.72F517
5.36	1,3-diphenyliso-benzofuran [$R_1 = R_3 = -Ph$]	H_2O	4.5×10^9	$(9.7 \pm 0.8) \times 10^{-5}$	rt	Ad-15	S=MB. k derived using k_d = *4.4×10^5 s^{-1} [1.1.3]. A solubilized in SDS micelles.	Gorm..76F247
5.36.1		H_2O	2.2×10^{10}		40	Ad-23	S = Py, A' = NaN_3. k derived using k_d = 5.0×10^5 s^{-1} [1.1]. S and A' solubilized in SDS micelles.	Miyo.78A174
5.36.2		H_2O	2.8×10^{10}		40	Ad-23	S = Py, A' = NaN_3. k derived using k_d = 5.0×10^5 s^{-1} [1.1]. S and A' solubilized in SDS micelles.	Miyo.78A174
5.36.3		H_2O	4.71×10^9	1.1×10^{-4}	25	Ad-15	S = MB. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [1.1]. S and A solubilized in SDS micelles.	Usui..78F061
5.36.4		H_2O	4.2×10^9	1.2×10^{-4}	25	Ad-15	S = Eos. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [1.1]. A solubilized in SDS micelles.	Usui..78F061
5.36.5		D_2O	8.4×10^8		rt	Ad-5	S=2-acetonaphthone, N_2 laser (337 nm). S and A solubilized in SDS micelles.	Gorm.78E144
5.36.6		MeOH	$\approx 7.7 \times 10^6$	$\approx 1.3 \times 10^{-2}$	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [1.3.6]. E_a = 2.9 kJ mol^{-1}.	Koch68F288
5.36.7		MeOH	$k_r = 9.1 \times 10^8$		25	Ad-17 A'd	S = RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 13.0. k_r derived using $k_r^{A'}$ = *7.0×10^7 dm^3 mol^{-1} s^{-1} [A3.16].	Youn..71F398
5.36.8		MeOH	$(7.0 \pm 1.0) \times 10^8$		rt	Ad-5	S = MB, ruby laser (694 nm).	Merk.71M325
5.36.9		MeOH	$(8.0 \pm 2.0) \times 10^8$		rt	Ad-5	S = MB, ruby laser (694 nm).	Merk.72F260
5.36.10		MeOH	$(1.3 \pm 0.1) \times 10^9$	$(6.7 \pm 0.3) \times 10^{-5}$	rt	Ad-8	S = MB, dye laser (610 nm).[a]	Youn..73F014
5.36.11		MeOH	$(1.2 \pm 0.4) \times 10^9$	$(8.1 \pm 1.5) \times 10^{-5}$	rt	Ad-8	S = RB, dye laser (583 nm).[a]	Youn..73F014
5.36.12		MeOH	$k_r = 6.13 \times 10^8$ *4.38×10^8	β_r = 2.27×10^{-4}	rt	Ad-14	S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [1.3] and $\phi_{isc} = 0.76$.	Olms.73F660

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.13	MeOH	$k_r = 1.4 \times 10^9$ *8.6×10^8		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 12.3. k_r derived using $k_r^{A'} = 1.1 \times 10^8$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.14	MeOH	1.4×10^9	$(7.0 \pm 2.6) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Brew74F646
5.36.15	MeOH	1.6×10^9	$(6.4 \pm 0.8) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Gorm..76F247
5.36.16	MeOH	$(1.0 \pm 0.1) \times 10^9$	1.1×10^{-4}	20	Ad-14	S = acridine orange. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.5*]. Complicated kinetic treatment.	Schm.76F105
5.36.17	MeOH	7.8×10^8 *5.6×10^8		rt	Ad-23	S = Py, A' = NaN_3. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*].	Miyo.78A174
5.36.18	MeOH	1.62×10^9	6.8×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.5*].	Usui..78F061
5.36.19	MeOH	1.64×10^9		25	Ad-5	S = MB, ruby laser (694 nm).	Usui..78F061
5.36.20	MeOH	1.55×10^9	7.1×10^{-5}	25	Ad-15	S = Ery. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.5*].	Usui..78F061
5.36.21	CH_2Cl_2	$k_r = 6.3 \times 10^8$ *5.1×10^8		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 7.3. k_r derived using $k_r^{A'} = 8.6 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.22	CH_2Cl_2	$(8.2 \pm 2.0) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.23	CH_2Cl_2	1.08×10^9		25	Ad-5	S = MB, ruby laser (694 nm).	Usui..78F061
5.36.24	CH_2Cl_2	1.6×10^9 *1.2×10^9	1.0×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 1.6 \times 10^4$ (*1.2×10^4) s^{-1} [*1.4*].	Usui..78F061
5.36.25	$CHCl_3$	$k_r = 1.4 \times 10^8$ *2.0×10^8		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 2.9. k_r derived using $k_r^{A'} = 4.9 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.26	$CHCl_3$	$(3.6 \pm 0.5) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.27	$CHCl_3$	7.0×10^8		25	Ad-5	S = MB, ruby laser (694 nm).	Usui..78F061
5.36.28	$CHCl_3$	9.0×10^8	1.0×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 9.0 \times 10^3$ s^{-1} [*1.5.2*].	Usui..78F061
5.36.29	CCl_4	$(2.6 \pm 0.4) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.30	CCl_4	1.1×10^8	1.2×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 1.4 \times 10^3$ s^{-1} [*1.8*].	Usui..78F061

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.31		CCl_4	$(8.0 \pm 2.4) \times 10^8$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
5.36.32		EtOH	4.4×10^8	$(1.8 \pm 1.0) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*].[a]	Brew74F646
5.36.33		EtOH	$(1.02 \pm .02) \times 10^9$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.34		EtOH	1.28×10^9	6.5×10^{-5}	25	Ad-15	S = Eos. k derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*].	Usui..78F061
5.36.35		glycol	1.5×10^9	3.16×10^{-4}	rt	Ad-8 16	S = MB or RB, dye laser. k derived using β and $k_D = 5.1 \times 10^{-5}$ s^{-1} at [DPBF] = 1.7×10^{-5} mol dm^{-3}.	Youn..73F014
5.36.36		$CHCl_2CH_3$	6.0×10^8		25	Ad-5	S = MB, ruby laser (694 nm).	Usui..78F061
5.36.37		$CHCl_2CH_3$	1.0×10^9	1.5×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 1.5 \times 10^4$ s^{-1} [*1.13*].	Usui..78F061
5.36.38		CH_2F-CH_2OH	$(5.1 \pm 3.9) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.39		$CHCl_2$-CH_2OH	$(5.7 \pm 1.1) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.40		CCl_3-CH_2OH	$(2.7 \pm 1.2) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.41		CF_3CH_2OH	1.7×10^8	$(1.36 \pm .47) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 2.3 \times 10^4$ s^{-1} [*1.16*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.42		CF_3CH_2OH	$k_r = 1.2 \times 10^8$		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. ($k_r/k_r^{A'}$) not reported. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.43		CF_3CH_2OH	$(6.0 \pm 1.3) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.44		CH_3CN	9.8×10^8	$(2.3 \pm 0.5) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = *2.55 \times 10^4$ s^{-1} [*1.17.2*].[a]	Brew74F646
5.36.45		CH_3CN	$k_r = 1.1 \times 10^9$ $*3.9 \times 10^8$		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 5.6. k_r derived using $k_r^{A'} = 2.0 \times 10^8$ ($*7.0 \times 10^7$) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.46		CH_3CN	$(6.6 \pm 0.7) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.47		$CHCl_2$-$CHCl_2$	4.4×10^8		25	Ad-5	S = MB, ruby laser (694 nm).	Usui..78F061
5.36.48		$CHCl_2$-$CHCl_2$	5.9×10^8	1.4×10^{-5}	25	Ad-15	S = MB. k derived using $k_d = 8.3 \times 10^3$ s^{-1} [*1.18*].[a]	Usui..78F061

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.49		CCl_2F–$CClF_2$	$k_r = 4.0 \times 10^7$		rt	Ad–36	$^1O_2$* from Nd–YAG CW laser (1065 nm). Measured ($k_r/k_{O_2}[O_2]$) = 1×10^4 dm^3 mol^{-1}. k_r derived using $k_{O_2}[O_2] = 4 \times 10^3$ s^{-1} (based on gas phase value for k_{O_2} of 1.3×10^3 dm^3 mol^{-1} s^{-1}).	Math.70F387
5.36.50		CCl_2F–$CClF_2$	$(1.0 \pm 0.2) \times 10^9$		rt	Ad–5	$^1O_2$* from pulsed Nd–YAG laser (1065 nm).	Math...74F102
5.36.51		CCl_2F–$CClF_2$	$k_r = (1.7 \pm 0.6) \times 10^8$		rt	Ad–5	$^1O_2$* from pulsed Nd–YAG laser (1065 nm). k_r derived using $k_A = 1.0 \times 10^9$ dm^3 mol^{-1} s^{-1} [*5.36.50*] and $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} [*15.1.4*].	Math...74F102
5.36.52		CCl_2F–$CClF_2$	$k_r = 7.6 \times 10^7$		rt	Ad–36	$^1O_2$* from Nd–YAG CW laser (1065 nm). Measured (k_r/k_{O_2}) = 2.8×10^4. k_r derived using $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} [*15.1.4*].	Math...74F102
5.36.53		CCl_2F–$CClF_2$	1.02×10^7 $k_r = 1.0 \times 10^7$ $k_q = 2.0 \times 10^5$	4.6×10^{-5}	25	Ad–34	$^1O_2$* from He/Ne laser (632.8 nm). Measured (k_q/k_r) = 0.02. k, k_r, and k_q derived using $k_d = 4.7 \times 10^2$ s^{-1} ([*1(a).2*];[*1(a).2.1*]).[b]	Evan.76F417
5.36.54		*i*–PrOH	4.5×10^8	$(1.1 \pm 0.3) \times 10^{-4}$	rt	Ad–15	S = MB. k derived using $k_d = 5.0 \times 10^4$ s^{-1} [*1.19*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.55		*i*–PrOH	$k_r = 6.1 \times 10^8$ *9.0×10^8		rt	Ad–17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 12.8. k_r derived using $k_r^{A'} = 4.8 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*]. Solvent contained 1% MeOH.	Brew74F646
5.36.56		*i*–PrOH	$(1.5 \pm 0.2) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.57		$(Me)_2CO$	6.5×10^8	$(4.8 \pm 1.3) \times 10^{-5}$	rt	Ad–15	S = MB. k derived using k_d = *3.1×10^4 s^{-1} [*1.22.2*].[a]	Brew74F646
5.36.58		$(Me)_2CO$	$k_r = 1.7 \times 10^9$ *6.6×10^8		rt	Ad–17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 9.4. k_r derived using $k_r^{A'} = 1.8 \times 10^8$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.59		$(Me)_2CO$	$(5.6 \pm 1.3) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.60		epibromohydrin	$(7.8 \pm 1.4) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm).[a]	Brew74F646

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.61		*n*-BuOH	$k_r = 7.3 \times 10^8$ *5.0×10^8	$\beta_r = 7.1 \times 10^{-5}$ *1.0×10^{-4}	25	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 7.47×10^{-2}. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Youn..71F398
5.36.62		*n*-BuOH	$(8.0 \pm 2.0) \times 10^8$	$(6.5 \pm 1.0) \times 10^{-5}$	rt	Ad-8	S = MB, dye laser (610 nm).[a]	Youn..73F014
5.36.63		*n*-BuOH	8.0×10^8	$(6.5 \pm 1.5) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.64		*n*-BuOH	$k_r = 8.3 \times 10^8$ *1.2×10^9		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 16.5 k_r derived using $k_r^{A'} = 5.0 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.65		*t*-BuOH	$k_r = 6.1 \times 10^8$ *4.2×10^8	$\beta_r = 4.9 \times 10^{-5}$ *7.2×10^{-5}	25	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($\beta_r/\beta_r^{A'}$(MeOH)) = 5.15×10^{-2}. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4×10^{-3}) mol dm^{-3} [*5.30.5*] and $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Youn..71F398
5.36.66		*t*-BuOH	$(5.7 \pm 0.8) \times 10^8$	$(5.3 \pm 0.7) \times 10^{-5}$	rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Youn..73F014
5.36.67		*t*-BuOH	2.3×10^8	$(1.3 \pm 0.6) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.68		*t*-BuOH	$k_r = 6.2 \times 10^8$ *1.2×10^9		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 17.3. k_r derived using $k_r^{A'} = 3.6 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.69		THF	$k_r = 8.3 \times 10^8$ *7.8×10^8		rt	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 11.1. k_r derived using $k_r^{A'} = 7.5 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.70		THF	$(5.0 \pm 1.8) \times 10^8$		rt	Ad-8	S = RB, dye laser (583 nm).[a]	Brew74F646
5.36.71		dioxane	$(1.21 \pm 0.16) \times 10^9$	$(2.4 \pm 0.8) \times 10^{-5}$	rt	Ad-8	S = MB, dye laser (610 nm).[a]	Youn..73F014
5.36.72		dioxane	$k_r = 3.1 \times 10^8$ *8.0×10^8		rt	Ad-17 A'd (sep)	S = RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 11.4. k_r derived using $k_r^{A'} = 2.7 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.73		dioxane	$(8.4 \pm 1.2) \times 10^8$		rt	Ad-8	S = RB, dye laser (583 nm).[a]	Brew74F646

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.74	ethyl acetate	$k_r = 3.5 \times 10^8$ *8.1×10^8		rt	Ad–17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 11.5. k_r derived using $k_r^{A'} = 3.0 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*].	Brew74F646
5.36.75	ethyl acetate	$(7.5 \pm 1.8) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.76	C_5H_5N	$k_r = 9.2 \times 10^8$		rt	Ad–17 A'd	S = A' = Rub. Measured ($k_r/k_r^{A'}$) = 21.9. k_r derived using $k_r^{A'}$ = *4.2×10^7 dm^3 mol^{-1} s^{-1} [*A3.17*].	Wils66F041
5.36.77	C_5H_5N	$(2.1 \pm 0.3) \times 10^9$	$(1.5 \pm 0.7) \times 10^{-5}$	rt	Ad–8	S = MB, dye laser (610 nm).[a]	Youn..73F014
5.36.78	C_5H_5N	$k_r = 4.8 \times 10^8$ *5.5×10^8		rt	Ad–17 A'd (sep)	S = RB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 7.86. k_r derived using $k_r^{A'} = 6.1 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.79	C_5H_5N	$(5.0 \pm 3.5) \times 10^8$		rt	Ad–8	S = RB, dye laser (583 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.80	n-C_6H_{14}	3.9×10^9 (est)	1.5×10^{-5}	rt	Pa–15	S = I_2. k estimated using k_d(cyclohexane) = 5.9×10^4 s^{-1} [*1.30*].	Olms.72F521
5.36.81	$C_6H_{11}OH$	2.1×10^8	$(3.0 \pm 1.6) \times 10^{-4}$	rt	Ad–15	S = MB. k derived using $k_d = 6.3 \times 10^4$ s^{-1} [*1.31*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.82	$C_6H_{11}OH$	$k_r = 6.5 \times 10^8$ *8.5×10^8		rt	Ad–17 A'd (sep)	S = MB, A' = DPF. Measured ($k_r/k_r^{A'}$) = 12.2. k_r derived using $k_r^{A'} = 5.3 \times 10^7$ (*7.0×10^7) dm^3 mol^{-1} s^{-1} [*A3.16*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.83	$C_6H_{11}OH$	$(1.4 \pm 2.2) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.84	C_6H_6	$(1.5 \pm 0.5) \times 10^9$		25	Ad–8	S = An, ruby laser (694 nm).	Farm.73F438
5.36.85	C_6H_6	$k_r = 7.0 \times 10^8$	$(6.0 \pm 0.5) \times 10^{-5}$	25	Ad–17 A'd	S = A' = Rub. Measured ($k_r/k_r^{A'}$) = 16.7. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.18*].	Stev..74F312
5.36.86	C_6H_6	4.7×10^8	$(8.5 \pm 4.2) \times 10^{-5}$	rt	Ad–15	S = MB. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.87	C_6H_6	$(3.5 \pm 1.3) \times 10^8$		rt	Ad–8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.88	C_6H_6	6.7×10^8	$(6.0 \pm 0.5) \times 10^{-5}$	25	Ad–15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev..74F649

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.89	C_6H_6	$k_r = 6.6 \times 10^8$ *5.0×10^8		25	Ad-17 A'd (sep)	S = self, A' = TME. Measured ($k_r/k_r^{A'}$) = 16.5 ± 1.5. k_r derived using $k_r^{A'} = 4.0 \times 10^7$ (*3.0×10^7) dm^3 mol^{-1} s^{-1} [*2.35.3, A3.2*].	Stev..74F649
5.36.90	C_6H_6	1.0×10^9	$(4.0 \pm 0.5) \times 10^{-5}$	rt	Ad-15	S = Rub. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Merk.78E036
5.36.91	C_6H_6	9.4×10^8		rt	Ad-5	S = Tetr,An,BP,benzil. k is based on data obtained using these sensitizers. 10 MeV pulse of electrons used to excite sensitizers.	Gorm..78E263
5.36.92	C_6H_6	6.7×10^8	6.0×10^{-5}	25	Pa-15	S = self. k derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Stev.79E106
5.36.93	C_6H_5Br	5.9×10^8	$(2.2 \pm 0.7) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.94	C_6H_5Br	$(5.4 \pm 1.3) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.95	methyl benzoate	2.8×10^8	$(8.9 \pm 1.3) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 2.5 \times 10^4$ s^{-1} [*1.37*]. Solvent contained 1% MeOH.[a]	Brew74F646
5.36.96	methyl benzoate	$(4.2 \pm 3.3) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm). Solvent contained 1% MeOH.[a]	Brew74F646
5.36.97	MeOH/H_2O (1:1) v:v	5.1×10^9	5.5×10^{-5}	rt	Ad-8 16	S = RB or MB, dye laser. k derived from β and k_D = $(3.7 \pm 1.2) \times 10^{-5}$ s^{-1} at [DPBF] = 1.7×10^{-5} mol dm^{-3}.	Youn..78F014
5.36.98	MeOH /glycol (1:1) v:v	1.9×10^9	6.3×10^{-5}	rt	Ad-8 16	S = MB or RB, dye laser. k derived from β and $k_D = (1.6 \pm 0.1) \times 10^{-5}$ s^{-1} at [DPBF] = 1.9×10^{-5} mol dm^{-3}.	Youn..73F014
5.36.99	$CHCl_3$ /MeOH (9:1) v:v	3.3×10^9 (est)	$(7.9 \pm 1.8) \times 10^{-5}$	rt	Ad-15	S = RB. k estimated using $k_d = 2.6 \times 10^4$ s^{-1} (calc).	Foot.76R071
5.36.100	$CHCl_3$ /MeOH (9:1) v:v	$k_r = 3.3 \times 10^9$		rt	Ad-14	S = RB. k_r derived using $\phi_{isc} = 0.66$ and $k_A = 3.3 \times 10^9$ dm^3 mol^{-1} s^{-1} [*5.36.99*].	Foot.76R071
5.36.101	CCl_4/MeOH (99:1) v:v	7.3×10^8		25	Ad-5	S = MB, flash photolysis.	Furu.78E238
5.36.102	CCl_4/MeOH (98:2) v:v	4.8×10^8		25	Ad-5	S = MB, flash photolysis.	Furu.78E238
5.36.103	CCl_4/MeOH (97:3) v:v	5.4×10^8		25	Ad-5	S = MB, flash photolysis.	Furu.78E238
5.36.104	CCl_4/MeOH (96:4) v:v	5.2×10^8		25	Ad-5	S = MB, flash photolysis.	Furu.78E238
5.36.105	CCl_4/MeOH (95:5) v:v	6.0×10^8		25	Ad-5	S = MB, flash photolysis.	Furu.78E238

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

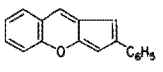
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.36.106		CCl_4/MeOH (94:6) v:v	$(2.5 \pm 0.2) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.107		CCl_4/MeOH (90:10) v:v	$(2.6 \pm 1.0) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.108		CCl_4/MeOH (86:14) v:v	$(2.6 \pm 0.2) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.109		CCl_4/MeOH (83:17) v:v	$(2.6 \pm 0.4) \times 10^8$		rt	Ad-8	S = MB, dye laser (610 nm).[a]	Brew74F646
5.36.110		CS_2/MeOH (98:2) v:v	$(3.0 \pm 0.5) \times 10^8$		rt	Ad-5	S = MB, flash photolysis.	Floo..73F334
5.36.111		C_6H_6/MeOH (4:1) v:v	$(9.1 \pm 2.0) \times 10^8$	$(4.1 \pm 0.8) \times 10^{-2}$	rt	Ad-8	S = MB, dye laser (610 nm).[a]	Youn..73F014
5.36.112		C_6H_6/MeOH (4:1) v:v	1.9×10^9	$(2.0 \pm 1.2) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 3.8 \times 10^4$ s^{-1} [*1.49*].[a]	Brew74F646
5.36.113		C_6H_6/MeOH (4:1) v:v	$k_r = 1.0 \times 10^9$		rt	Ad-17 A'd (sep)	S = MB, A' = DPF. ($k_r/k_r^{A'}$) unreported.[a]	Brew74F646
5.36.114		C_6H_5Br /MeOH (4:1) v:v	4.6×10^8	$(9.3 \pm 5.1) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 4.3 \times 10^4$ s^{-1} [*1.50*].[a]	Brew74F646
5.36.115		C_6H_5Br /MeOH (4:1) v:v	$(7.0 \pm 1.3) \times 10^8$	$(6.2 \pm 1.0) \times 10^{-5}$	rt	Ad-8	S = MB, dye laser (610 nm).[a]	Youn..73F014
		For more relative rates see		2.35.10, 3.65, 8.2.9, 8.7.6, 8.8.7, 14.32.7.				
5.37	1,3-diphenyl-5,6-dimethylisobenzofuran [$R_1 = R_3 = -Ph$, $R_5 = R_6 = -Me$]	MeOH	$k_r = 5.24 \times 10^8$ *3.74×10^8		rt	Ad-14	S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*] and $\phi_{isc} = 0.76$ [71M325].	Olms.73F660
5.38	1,3,4,7-tetraphenylisobenzofuran [$R_1 = R_3 = R_4 = R_7 = -Ph$]	MeOH	$k_r = 6.62 \times 10^8$ *4.73×10^8		rt	Ad-14	S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*] and $\phi_{isc} = 0.76$ [71M325].	Olms.73F660
5.39	1,3,4,5,6,7-hexaphenylisobenzofuran [$R_1 = R_3 = R_4 = R_5 = R_6 = R_7 = -Ph$]	MeOH	$k_r = 6.88 \times 10^8$ *4.91×10^8		rt	Ad-14	S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*] and $\phi_{isc} = 0.76$ [71M325].	Olms.73F660
5.40	2-phenylbenzo[b]-cyclopentadieno[e]-pyran 	C_6H_6	7.8×10^5	$(5.4 \pm 0.6) \times 10^{-2}$	rt	Ad-15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Timp..78F438
			COMPOUNDS 5.41 - 5.44 : 					
5.41	1-*t*-butylpyrrole [$R_1 = -(t\text{-Bu})$]	MeOH	3.9×10^7 *3.2×10^7	9.7×10^{-4}	rt	Od-?	S = MB. k derived using $k_d = 3.8 \times 10^4$ (*3.1×10^4) s^{-1} [*1.22*].	Ligh.75F652
5.41.1		$(Me)_2CO$	8.3×10^8	1.2×10^{-4}	rt	Od-?	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.75F652

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

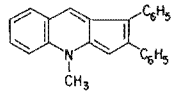
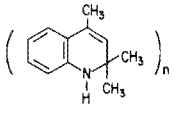
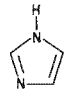
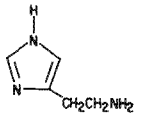
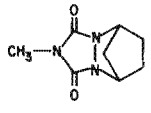
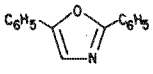
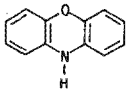
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.42	2-*t*-butylpyrrole [R_2 = -(*t*-Bu)]	MeOH	1.1×10^8	9.3×10^{-4}	rt	Od-?	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.75F652
5.42.1		$(Me)_2CO$	4.2×10^7 $*3.4 \times 10^7$	9.0×10^{-4}	rt	Od-?	S = MB. k derived using $k_d = 3.8 \times 10^4$ ($*3.1 \times 10^4$) s^{-1} [*1.22*].	Ligh.75F652
5.43	3-*t*-butylpyrrole [R_3 = -(*t*-Bu)]	MeOH	1.3×10^8	7.8×10^{-4}	rt	Od-?	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.75F652
5.43.1		$(Me)_2CO$	2.9×10^7 $*2.4 \times 10^7$	1.3×10^{-3}	rt	Od-?	S = MB. k derived using $k_d = 3.8 \times 10^4$ ($*3.1 \times 10^4$) s^{-1} [*1.22*].	Ligh.75F652
5.44	2,5-dimethylpyrrole [$R_2 = R_5$ = -Me]	MeOH	6.25×10^5	1.6×10^{-1}	20	Od-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 7.1 kJ mol^{-1}.	Koch68F288
5.45	pyridine 	CCl_4	$(1.7 \pm 2.2) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
5.46	1,2-diphenyl-4*H*-4-methylcyclopenta-dieno[b]quinoline 	C_6H_6	3.0×10^6	$(1.40 \pm 0.25) \times 10^{-2}$	rt	Ad-15	S = self. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Timp..78F438
5.47	quinoline 	EtOH	$< 1 \times 10^9$ (est)		0	Od-23	S = MB, A' = DMF. No measurable effect.	Dall..72F518
5.48	Permanax 45 	EtOH	9.6×10^8		0	Od-23	S = MB, A' = DMF. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*] and $k_{A\cdot} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518
5.49	imidazole 	H_2O (pH 7.1)	4×10^7		25	Od-19	S = phenosafranine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
5.49.1		H_2O (pH 7.0)	2.0×10^7		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in triton X-100 micelles (1% by volume).	Barb.78A278
5.49.2		H_2O (pH 7.0)	2.9×10^7		rt	Od-19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in triton X-100 micelles (2% by volume).	Barb.78A278

TABLE 5. Rate constants for the interaction of singlet molecular oxygen with furans, pyrroles, and related compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	($\beta = k_d/k$) /mol dm^{-3}	t /°C	Method	Comments	Ref.
5.49.3		H_2O (pH 7.0)	3.9×10^7		rt	Od–19	S = chlorophyll-a, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in triton X-100 micelles (5% by volume).	Barb.78A278
5.49.4		H_2O (pH 7.0)	3.6×10^7		rt	Od–19	S = hematoporphyrin, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in triton X-100 micelles (1% by volume).	Barb.78A278
5.49.5		H_2O (pH 7.0)	3.4×10^7		rt	Od–19	S = hematoporphyrin, Q = N_3^-. k derived using $k_Q = 2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Barb.78A278
5.50	histamine 	H_2O (pH 7.1)	2.8×10^7		25	Od–19	S = phenosafranine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
5.50.1		H_2O	2.0×10^8	2.5×10^{-3}	25	Ad–15	S = MB. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Usui..78F061
5.50a	4-methyl-3,5-dioxotriazolo-norbornane 	C_6H_6 /MeOH (3:1) v:v	$< 3 \times 10^5$ (est)		25	A'd–20	S=RB. A' = cyclohexene. k estimated using $\beta_{A'} = 3.1$ mol dm^{-3} [*2.54.3*] and $k_d = 6.25 \times 10^4$ s^{-1}.	Kret.78F586
5.51	2,5-diphenyloxazole 	H_2O/D_2O (1:1) Mole %	1.6×10^8 (est)	2.2×10^{-3}	25	Ad–15	S = MB. k estimated using $k_d = 2.75 \times 10^5$ s^{-1} (calc). A solubilized in DTAC micelles.	Usui..78F061
5.51.1		H_2O/D_2O /MeOH (2:5:3) Mole %	1.6×10^8 (est)	1.6×10^{-3}	25	Ad–15	S = MB. k estimated using $k_d = 2.58 \times 10^5$ s^{-1} (calc).	Usui..78F061
5.52	phenoxazine 	C_6H_5Br /MeOH (2:1) v:v	1.0×10^7 (est)		rt	A'd–23	S = A' = Rub. k estimated using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.89 \times 10^4$ s^{-1} (calc).	Rose..77F240

[a]The errors reported on k or β are 90 % confidence limits.
[b]This value of k_d is an average of the k_d values reported under the given entries.

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
6.1	ethylamine $C_2H_5NH_2$	CCl_2F–$CClF_2$	$(3.1 \pm 0.6) \times 10^4$ (est)		23	A′d–37	$^1O_2$* from Nd–YAG CW laser (1065 nm), A′ = tetracyclone. Measured (k/k_{O_2}) = $(2.4 \pm 0.5) \times 10^1$. k estimated using $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value [71E034]).	Math.72F513
6.2	propylamine $CH_3CH_2CH_2NH_2$	$CHCl_3$	$(2.3 \pm 0.3) \times 10^5$		rt	A′d–33	S = A′ = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^{-3} mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.3	isopropylamine $CH_3CH(CH_3)NH_2$	MeOH	8.5×10^4	1.18	rt	A′d–16	S = MB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.3.1		MeOH	5.3×10^4	1.87	rt	A′d–16	S = RB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.3.2		MeOH	5.0×10^4	2.02	rt	A′d–16	S = RB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.4	butylamine $CH_3(CH_2)_2CH_2NH_2$	$CHCl_3$	$(2.4 \pm 0.3) \times 10^5$		rt	A′d–33	S = A′ = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.4.1		EtOH	$< 1 \times 10^9$ (est)		0	Od–23	S = MB, A′ = DMF. No measurable effect.	Dall..72F518
6.5	isobutylamine $CH_3CH(CH_3)CH_2NH_2$	$CHCl_3$	$(4.1 \pm 0.5) \times 10^5$		rt	A′d–33	S = A′ = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.6	*t*-butylamine $CH_3C(CH_3)_2NH_2$	MeOH	3.7×10^4	2.67	rt	A′d–16	S = MB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.6.1		MeOH	7.4×10^5	1.36×10^{-1}	rt	A′d–16	S = RB, A′ = DPBF k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.7	cyclohexylamine $C_6H_{11}NH_2$	MeOH	8.9×10^4	1.12	rt	A′d–16	S = RB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.8	benzylamine $C_6H_5CH_2NH_2$	MeOH	2.9×10^5	3.44×10^{-1}	rt	A′d–16	S = RB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.8.1		MeOH	1.2×10^5	8.1×10^{-1}	rt	A′d–16	S = MB, A′ = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.8.2		EtOH	$< 1 \times 10^9$ (est)		0	Od–23	S = MB, A′ = DMF. No measurable effect.	Dall..72F518

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

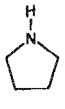
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.9	2-phenyl-ethylamine $C_6H_5CH_2CH_2NH_2$	MeOH	6.5×10^5	1.54×10^{-1}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.9.1		MeOH	1.7×10^5	5.83×10^{-1}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.10	3-phenylpropyl-amine $C_6H_5CH_2CH_2CH_2NH_2$	MeOH	8.8×10^4	1.13	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.10.1		MeOH	7.6×10^4	1.32	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.11	4-phenylbutyl-amine $C_6H_5CH_2(CH_2)_2CH_2NH_2$	MeOH	1.0×10^5	9.8×10^{-1}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.12	diethylamine $(C_2H_5)_2NH$	MeOH	8.8×10^5	1.13×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.12.1		MeOH	2.1×10^6	4.77×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.12.2		$CHCl_3$	$(1.5 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.12.3		CCl_2F-$CClF_2$	$(5.7 \pm 0.9) \times 10^5$ (est)		23	A'd-37	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured $(k/k_{O_2}) = (4.4 \pm 0.7)$ x 10^2. k estimated using $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value [71E034]).	Math.72F513
6.12.4		C_6H_6 /MeOH (3:1) v:v	2.4×10^6		25	A'd-20	S = RB, A' = cyclohexene. k derived using $\beta_{A'} = 3.1$ mol dm^{-3} [*2.54.3*] and k_d = 6.25×10^4 s^{-1}.	Kret.78F586
6.13	dipropyl-amine $(CH_3CH_2CH_2)_2NH$	$CHCl_3$	$(1.8 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.14	diisopropyl-amine $((CH_3)_2CH)_2NH$	$CHCl_3$	$(1.8 \pm 0.2) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.15	tetrahydro-pyrrole 	MeOH	3.4×10^5	2.9×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

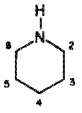
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.15.1		MeOH	2.4×10^6	4.2×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
				COMPOUNDS 6.16 - 6.18 : 				
6.16	piperidine	MeOH	4.1×10^5	2.44×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.16.1		MeOH	1.0×10^6	9.8×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.16.2		$CHCl_3$	$(5.8 \pm 0.6) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.17	2,6-dimethyl-piperidine [$R_2 = R_6$ = -Me]	$CHCl_3$	$(3.0 \pm 0.3) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.18	2,2,6,6-tetramethyl-4-hydroxypiperidine [$R_2 = R_2 = R_6 = R_6$ = -Me, R_4 = -OH]	$CHCl_3$	$< 2.0 \times 10^5$ (est)		rt	A'd-33	S = A' = Rub. No measurable effect.	Monr77F486
6.18.1		C_6H_6 /EtOH (8:1) v:v	5×10^5		22	A'd-23	S = RB, A' = Tetr. k derived using $k_{A'}$ = 7×10^7 dm^3 mol^{-1} s^{-1} and $k_d = 3 \times 10^4$ s^{-1}.	Ivan....75F445
6.18.2		C_6H_6 /EtOH (8:1) v:v	$k_r = 2.9 \times 10^3$ *4.9×10^2		22	Pa-17 A'd	S = RB, A' = Tetr, P = nitroxy radicals. Measured ($k_r/k_r^{A'}$) = 4.1×10^{-5}. k_r derived using $k_r^{A'} = 7 \times 10^7$ (*1.2×10^7) dm^3 mol^{-1} s^{-1} [*A3.13*].	Ivan....75F445
6.19	di(2-hydroxyethyl)-methylamine $CH_3N(CH_2CH_2OH)_2$	$CHCl_3$	$(2.1 \pm 0.3) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.20	*N,N*-dimethyl-formamide $HCON(CH_3)_2$	EtOH	$k_r = 3.0 \times 10^2$		rt	Pa-19	S = RB. k_r derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*] and (k_q/k_r) = (not reported). k_r derived assuming a singlet oxygen mechanism.	Zolo..75F655

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.21	*N,N*-dimethyliso-butenylamine $(CH_3)_2C = CHN(CH_3)_2$	C_6H_6	$k_r = 3.1 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 10.3 ± 1.0. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.1		C_6H_6 /Me_2SO (4:1) v:v	$k_r = 3.2 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 10.8 ± 0.05. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.2		C_6H_6 /Me_2SO (3:2) v:v	$k_r = 2.3 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 7.6 ± 0.1. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.3		C_6H_6 /Me_2SO (1:4) v:v	$k_r = 2.7 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 9.1 ± 0.3. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.4		C_6H_6 /CH_3CN (4:1) v:v	$k_r = 2.3 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 7.8 ± 0.12. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.5		C_6H_6 /CH_3CN (1:19) v:v	$k_r = 2.8 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 9.4 ± 0.2. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.6		C_6H_6 /pentane (1:19) v:v	$k_r = 2.1 \times 10^8$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 7.1 ± 0.2. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.7		C_6H_6 /MeOH (3:7) v:v	$k_r = 8.7 \times 10^7$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 2.9 ± 0.1. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.21.8		C_6H_6 /MeOH (1:19) v:v	$k_r = 6.6 \times 10^7$		rt	Ad-17 A'd	S = ZnTPP, A' = TME. Measured ($k_r/k_r^{A'}$) = 2.2 ± 0.15. k_r derived using $k_r^{A'} = *3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*A3.2*].	Foot..75F656
6.22	trimethylamine $(CH_3)_3N$	MeOH	1.5×10^7	6.69×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F519
6.23	triethylamine $(C_2H_5)_3N$	MeOH	1.3×10^7	7.6×10^{-3}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn.72F514
6.23.1		MeOH	7.4×10^6	1.35×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F519
6.23.2		MeOH	1.0×10^7	9.7×10^{-3}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Youn....73E061

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.23.3		$CHCl_3$	$(6.5 \pm 0.7) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.23.4		CCl_2F-$CClF_2$	$(2.1 \pm 0.3) \times 10^6$ (est)		23	A'd-37	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured $(k/k_{O_2}) = (1.6 \pm 0.3)$ x 10^3. k estimated using $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value [71E034]).	Math.72F513
6.23.5		EtOH	$k_r = 2.7 \times 10^6$	3.1×10^{-1}	rt	Pa-19	S = RB. k_r derived using $k_d = 8.3 \times 10^4$ s^{-1} [*1.10*] and (k_q/k_r) = 9.3.	Zolo..75F655
6.23.6		C_5H_5N	$k_r = 2.2 \times 10^7$	2.7×10^{-3}	rt	Od-14 27	S = RB, A' = 2M2P. k derived using k_d = *5.9 $\times 10^4$ s^{-1} [*1.29.1*].	Smit72F512
6.23.7		C_5H_5N	$k_q = 2.0 \times 10^8$	2.9×10^{-4}	rt	Od-14 27	S = RB, A' = 2M2P. k derived using k_d = *5.9 $\times 10^4$ s^{-1} [*1.29.1*].	Smit72F512
6.23.8		C_5H_5N	1.4×10^8	4.2×10^{-4}	rt	Od-20	S = RB, A' = 2M2P. k derived using k_d = *5.9 $\times 10^4$ s^{-1} [*1.29.1*].	Smit72F512
6.24	diethyl(2-hydroxyethyl)amine $(C_2H_5)_2NCH_2CH_2OH$	$CHCl_3$	$(3.0 \pm 0.3) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.25	diethyl(2-methoxyethyl)amine $(C_2H_5)_2NCH_2CH_2OCH_3$	$CHCl_3$	$(3.8 \pm 0.4) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.26	diethyl(2-cyano-ethyl)amine $(C_2H_5)_2NCH_2CH_2CN$	$CHCl_3$	$(2.7 \pm 0.3) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.27	diethyl(7-amino-heptyl)amine $(C_2H_5)_2NCH_2(CH_2)_5CH_2NH_2$	$CHCl_3$	$(6.1 \pm 0.7) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.28	tributylamine $(CH_3(CH_2)_2CH_2)_3N$	$CHCl_3$	$(5.8 \pm 0.6) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

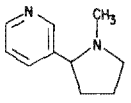
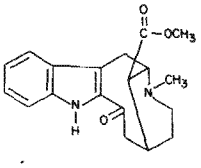
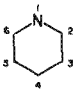
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.28.1		EtOH	$\leqslant 1 \times 10^9$ (est)		0	Od-23	S = MB, A′ = DMF. No measurable effect.	Dall..72F518
6.29	di(2-hydroxy-ethyl)-*t*-butylamine $(CH_3)_3CN(CH_2CH_2OH)_2$	$CHCl_3$	$(1.1 \pm 0.2) \times 10^6$		rt	A′d-33	S = A′ = Rub. *k* derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.30	nicotine 	MeOH	4.4×10^5	2.27×10^{-1}	15	Od-?	S = RB, A′ = α-terpinene. *k* derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. Found $k_q = 5.4\ k_r$.	Sche.58F004
6.31	dregamine 	C_6H_6	2.7×10^7	1.47×10^{-3}		Ad-15	S = ZnTPP. *k* derived using k_d = *4.0×10^4 s^{-1} [*1.32.9*].	Herl.78F474
6.31.1		MeOH /C_6H_6 (2:1)	4.0×10^7 (est)	2.02×10^{-3}		Ad-15	S = ZnTPP. *k* derived using $k_d = 8.0 \times 10^4$ s^{-1} (calc).	Herl.78F474
	COMPOUNDS 6.32 – 6.36 : 							
6.32	1-methyl-piperidine [R_1 = -Me]	$CHCl_3$	$(5.3 \pm 0.6) \times 10^7$		rt	A′d-33	S = A′ = Rub. *k* derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.33	4-hydroxy-1,2,-2,6,6-pentamethyl-piperidine [$R_1 = R_2 = R_2 = R_6 = R_6$ = -Me, R_4 = -OH]	$CHCl_3$	$(9.2 \pm 1.0) \times 10^7$		rt	A′d-33	S = A′ = Rub. *k* derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.33.1		CH_2Cl_2	5×10^7		22	A′d-?	Method not given.	Ivan....75F445
6.33.2		CH_2Cl_2	8.6×10^7	1.4×10^{-4}	rt	A′d-19	S = A′ = Tetr. *k* derived using $k_{A'} = 3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.62*].	Byst.75F654
6.33.3		C_6H_6/EtOH (8:1)v:v	$k_r = 2.3 \times 10^3$ *4.0×10^2		22	Pa-17 A′d	S = RB, A′ = Tetr, P = nitroxy radicals. Measured ($k_r/k_r^{A'}$) = 3.3×10^{-5}. k_r derived using $k_r^{A'} = 7 \times 10^7$ (*1.2×10^7) dm^3 mol^{-1} s^{-1} [*A3.13*].	Ivan....75F445

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

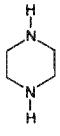
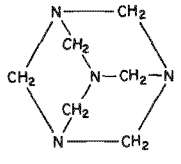
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.34	*N*-(2-hydroxyethyl)-2,2,6,6-tetramethylpiperidine [$R_2 = R_2 = R_6 = R_6 = -Me$, $R_1 = -CH_2CH_2OH$]	$CHCl_3$	$< 2 \times 10^5$ (est)		rt	Ad'-33	S = A' = Rub. No measurable effect.	Monr77F486
6.35	*N*-(2-acetoxyethyl)-2,2,6,6-tetramethylpiperidine [$R_2 = R_2 = R_6 = R_6 = -Me$, $R_1 = -CH_2CH_2OCOCH_3$]	$CHCl_3$	$< 2 \times 10^5$ (est)		rt	A'd-33	S = A' = Rub. No measurable effect.	Monr77F486
6.36	1-cyclohexylpiperidine [$R_1 = -C_6H_{11}$]	MeOH	5.1×10^7	1.98×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]	Mart72F519
6.37	*N*-allylurea $CH_2 = CHCH_2NHCONH_2$	H_2O (pH 7.1)	$< 2 \times 10^5$		25	Od-19	S = phenosafranine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78F020
6.38	quinuclidine 	MeOH	2.0×10^6	5.1×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.39	piperazine 	MeOH	1.4×10^6	7.3×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061
6.40	1,4-diazabicyclo[2.2.2]octane (DABCO) 	MeOH	1.5×10^7	6.5×10^{-3}	rt	P'a-20	S = ZnTPP, A' = 2M2P. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Foot..72F028
6.40.1		MeOH	8.1×10^6	1.23×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn.72F514
6.40.2		$CHCl_3$	$(5.2 \pm 0.6) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*] and $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*].	Monr77F486
6.40.3		CCl_4	$(7.0 \pm 2.1) \times 10^6$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
6.40.4		CS_2	2.9×10^7	1.7×10^{-4}	rt	P'a-20	S = ZnTPP, A' = 2M2P. k derived using $k_d = 5.0 \times 10^3$ s^{-1} [*1.9*].	Foot..72F028

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.40.5		EtOH	1.4×10^7		rt	Ad-23	S = RB, A′ = hexamethylenedithiocarbamate. Measured $k_A/(k_d + k[A]) = 58$ at $[A] = 4.48 \times 10^{-4}$ mol dm^{-3}. k derived using $k_{A'} = 2.7 \times 10^8$ dm^3 mol^{-1} s^{-1} [*11.42*] and $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*].	Yama..72F116
6.40.6		EtOH	$\leqslant 1 \times 10^9$ (est)		0	Od-23	S = MB, A′ = DMF. No measurable effect.	Dall..72F518
6.40.7		EtOH	3.11×10^7 (est)		rt	A′d-19	S = RB, A′ = chlorophyll-a. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
6.40.8		*n*-BuOH	4.5×10^6	1.15×10^{-2}	rt	A′d-16	S = RB, A′ = DPBF. k derived using $k_d = 5.2 \times 10^4$ s^{-1} [*1.24*].	Youn.72F514
6.40.9		C_5H_5N	2.6×10^8	2.3×10^{-4}	rt	Od-20	S = RB, A′ = 2M2P. k derived using $k_d = *5.9 \times 10^4$ s^{-1} [*1.29.1*].	Smit72F512
6.40.10		C_5H_5N	1.8×10^8	3.2×10^{-4}	rt	Od-21	S = RB, A′ = triethylamine. k derived using $k_d = *5.9 \times 10^4$ s^{-1} [*1.29.1*].	Smit72F512
6.40.11		C_5H_5N	$(3.1 \pm 2.0) \times 10^8$		rt	A′d-23	S = A′ = Rub. k derived using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = *6.0 \times 10^4$ s^{-1} [*1.29.1*].	Fahr...74R112
6.40.12		C_6H_6	4.2×10^7	9.6×10^{-4}	rt	P′a-20	S = ZnTPP, A′ = 2M2P. k derived using $k_d = *4.0 \times 10^4$ s^{-1} [*1.32.9*].	Foot..72F028
6.40.13		C_6H_6	1.4×10^7	$(2.9 \pm 0.1) \times 10^{-3}$	rt	Ad-16	S = A′ = 1,2-diphenyl-4H-4-methyl cyclopentadieno-[b]quinoline. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Timp..78F438
6.40.14		$C_6H_5CH_3$	1.9×10^8	2.1×10^{-4} (est)	rt	A′d-23	S = A′ = Rub. β estimated using $\beta_{A'} = 9.1 \times 10^{-4}$ mol dm^{-3} [*3.63.25*]. k derived using $k_d = 4.0 \times 10^4$ s^{-1} [*1.36*].	Ouan.68F285
6.40.15		$C_6H_6CH_3$	6.7×10^8 (est)		rt	A′d-25	S = A′ = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_{A'} = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
6.40.16		C_6H_5Br	8.7×10^8	1.5×10^{-5} (est)	rt	A′d-23	$^1O_2$* from electric discharge, A′ = DPBF. β estimated using $\beta_{A'} = 2.2 \times 10^{-5}$ mol dm^{-3}. k derived using $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Ouan.68F285

TABLE 6. Rate constants for the interaction of singlet oxygen with aliphatic and cyclic amines — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
6.40.17		C_6H_5Br	2.6×10^7		0	A'd-33	$^1O_2$* from microwave discharge, A' = Rub. Measured $k/[k_d/[A'] + k_{A'}] = 0.2$ at [A'] = 1.5×10^{-4} mol dm^{-3}. k derived using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Guil.73F333
6.40.18		o-$C_6H_4Cl_2$	5.2×10^6 (est)	2.5×10^{-3} (est)	rt	A'd-23	$^1O_2$* from electric discharge, A' = Rub. β estimated using $\beta_{A'} = 4.0 \times 10^{-4}$ mol dm^{-3} [*3.63.24*]. k estimated using $k_d(C_6H_5Br) = 1.3 \times 10^4$ s^{-1} [*1.34*].	Ouan.68F28
6.40.19		i-octane	3.0×10^7 (est)		25	A'd-23	S = A' = Rub. k estimated using $k_d = 4.7 \times 10^7$ s^{-1} [*1(a).6.1*] and $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..74F341
6.40.20		C_6H_6 /MeOH (4:1) v:v	1.6×10^7		25	P'a-20	S = MB, A' = 2M2P. k derived using $\beta_{A'} = 4.0 \times 10^{-2}$ mol dm^{-3} and $k_d = 1.0 \times 10^4$ s^{-1}.	Foot....70F734
6.40.21		CH_2Cl_2 /MeOH /C_5H_5N (90:5:5) v:v:v	3.3×10^7 (est)		25	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_d = 8 \times 10^3$ s^{-1} and $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..74F341
6.40.22		CH_2Cl_2 /MeOH /C_5H_5N (94:3:3) v:v:v	3.3×10^7 (est)		25	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl...72F319
6.40.23		i-octane /MeOH /C_5H_5N (94:3:3) v:v:v	3.5×10^7 (est)		25	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 5.0 \times 10^4$ s^{-1}.	Carl...72F319
6.40.24		i-octane /MeOH /C_5H_5N (90:5:5) v:v:v	3.9×10^7 (est)		25	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_d = 4.7 \times 10^4$ s^{-1} and $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..74F341
6.41	hexamethylene-tetramine 	MeOH	1.7×10^5	6.0×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
6.41.1		MeOH	2.2×10^5	4.6×10^{-1}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Youn....73E061

[a] β has been corrected for contributions due to quenching of ^{3}S by substrate A.

TABLE 7. Rate constants for the interaction of singlet oxygen with aromatic amines

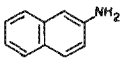
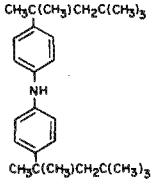
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
7.1	aniline $C_6H_5NH_2$	?	1.2×10^8		rt	A'd-20	S = Eos,Ery, or RB, A' = TME. Measured ($k_{A'}/k$) = 3.35×10^{-1}. k derived using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*2.35.3*].	Pouy.71F299
7.1.1		?	1.1×10^8		rt	A'd-20	S = self, A' = TME. Measured ($k_{A'}/k$) = 3.64×10^{-1}. k derived using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*2.35.3*].	Pouy.71F299
7.2	2-amino-naphthalene 	EtOH	9.6×10^8		0	Od-23	S = MB, A' = DMF. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*] and $k_{A'} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518
7.3	*N*-methylaniline $C_6H_5NHCH_3$	MeOH	3.0×10^7	3.4×10^{-3}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.3.1		CCl_2F-$CClF_2$	$(3.8 \pm 0.3) \times 10^4$ (est)		23	A'd-37	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured (k/k_{O_2}) = $(2.9 \pm 0.2) \times 10^1$. k estimated using $k_{O_2} = 1.3 \times 10^3$ dm^3 mol^{-1} s^{-1} (gas phase value [71E034]).	Math.72F513
7.4	diphenylamine $(C_6H_5)_2NH$	MeOH	7.9×10^6	1.26×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
7.4.1		MeOH	6.7×10^6	1.5×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.5	4,4'-di-*t*-octyl-diphenylamine 	C_6H_6/EtOH (8:1) v:v	7.3×10^6 (est)		22	A'd-23	S = RB, A' = Tetr, A'' = Ni(II) dibutyldithiocarbamate. k estimated using $k_{A''} = 1.6 \times 10^9$ dm^3 mol^{-1} s^{-1} [*10.17.12*], $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1}, and $k_d = 3 \times 10^4$ s^{-1} (calc).	Ivan....75F445
7.5.1		C_6H_6/EtOH (8:1) v:v	$k_r = 2.6 \times 10^4$ *4.4×10^3		22	Pa-17 A'd	S = RB, A' = Tetr, P = nitroxy radicals. Measured ($k_r/k_r^{A'}$) = 3.7×10^{-4}. k_r derived using $k_r^{A'} = 7 \times 10^7$ (*1.2×10^7) dm^3 mol^{-1} s^{-1} [*A3.13*].	Ivan....75F445

TABLE 7. Rate constants for the interaction of singlet oxygen with aromatic amines — Continued

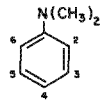
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
				COMPOUNDS 7.6 - 7.13 : 				
7.6	*N,N*-dimethyl-aniline	MeOH	1.0×10^8	9.93×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
7.6.1		MeOH	1.3×10^8	$(7.6 \pm 0.9) \times 10^{-4}$	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.6.2		MeOH	$(7.3 \pm 0.8) \times 10^7$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn..73F014
7.6.3		MeOH(?)	3.5×10^6	2.9×10^{-2}	rt	A'd-?	S = RB, A' = DMF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Davi.77F055
7.6.4		CCl_2F-$CClF_2$	$(2.0 \pm 0.4) \times 10^5$ (est)		23	A'd-37	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured $(k/k_{O_2}) = (1.6 \pm 0.3) \times 10^2$. k estimated using k_{O_2} = 1.3×10^3 dm^3 mol^{-1} s^{-1} (gas phase value [71E034]).	Math.72F513
7.6.5		C_5H_5N	1.0×10^8 *1.9×10^8	5.9×10^{-4}	rt	Od-20	S = RB, A' = 2M2P. k derived using $\beta_{A'}$ = 4.3×10^{-2} mol dm^{-3} and $k_d = 3.1 \times 10^4$ (*5.9×10^4) s^{-1} [*1.29*].	Smit..75F166
7.7	*m*-chloro-*N,N*-dimethylaniline [R_3 = -Cl]	MeOH	2.2×10^6	4.52×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
7.7.1		MeOH	1.4×10^7	7.15×10^{-3}	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.7.2		MeOH	$(1.1 \pm 0.1) \times 10^7$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.8	*p*-bromo-*N,N*-dimethylaniline [R_4 = -Br]	MeOH	5.7×10^6	1.76×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
7.8.1		MeOH	3.2×10^7	$(3.1 \pm 0.8) \times 10^{-3}$	rt	A'd-16	S = RB, A' =DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.8.2		MeOH	$(1.7 \pm 0.4) \times 10^7$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.9	*p*-methyl-*N,N*-dimethylaniline [R_4 = -Me]	MeOH	2.1×10^8	4.68×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F51

TABLE 7. Rate constants for the interaction of singlet oxygen with aromatic amines — Continued

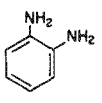
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
7.9.1		MeOH	1.8×10^8	$(5.5 \pm 0.3) \times 10^{-4}$	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Youn....73E061
7.9.2		MeOH	$(1.2 \pm 0.4) \times 10^8$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.10	*p*-cyano-*N*,*N*-dimethylaniline [R_4 = -CN]	MeOH	4.0×10^6	2.51×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F51
7.10.1		MeOH	2.0×10^6	5.0×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Youn....73E061
7.10.2		MeOH	$(5.7 \pm 0.1) \times 10^5$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.11	*p*-(*N*,*N*-dimethylamino)-benzaldehyde [R_4 = -CHO]	MeOH	2.2×10^6	4.58×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F519
7.11.1		MeOH	2.7×10^6	3.7×10^{-2}	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Youn....73E061
7.11.2		MeOH	$(1.2 \pm 0.6) \times 10^6$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn...74F640
7.12	*m*-methoxy-*N*,*N*-dimethyl-aniline [R_3 = -OCH_3]	MeOH	1.4×10^8	7.07×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F519
7.12.1		MeOH	6.7×10^7	$(1.5 \pm 0.4) \times 10^{-3}$	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Youn....73E061
7.12.2		MeOH	$(4.8 \pm 0.4) \times 10^7$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.13	*p*-methoxy-*N*,*N*-dimethyl-aniline [R_4 = -OCH_3]	MeOH	5.5×10^8	1.84×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Mart72F519
7.13.1		MeOH	2.1×10^8	$(4.7 \pm 1.1) \times 10^{-4}$	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].[a]	Youn....73E061
7.13.2		MeOH	$(1.8 \pm 0.4) \times 10^8$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn....74F640
7.14	*o*-phenylenediamine 	EtOH	3.4×10^9		0	Od-23	S = MB, A' = DMF. k derived using $k_d = *7.9 \times 10^4$ s^{-1} [*1.10.3*] and $k_{A'} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518

TABLE 7. Rate constants for the interaction of singlet oxygen with aromatic amines — Continued

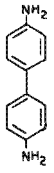
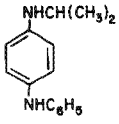
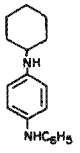
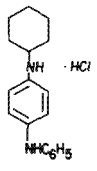
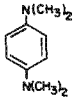
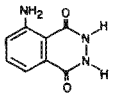
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
7.15	4,4′-diamino-biphenyl 	EtOH	3.0×10^9		0	Od–23	S = MB, A′ = DMF. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*] and $k_{A'} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518
7.16	1-isopropylamino-4-phenylamino-benzene 	EtOH	6.7×10^9		0	Od–23	S = MB, A′ = DMF. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*] and $k_{A'} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518
7.16.1		*i*-octane	3.3×10^8 (est)		rt	A′d–23	S = A′ = Rub. k estimated using $k_d = 4 \times 10^4$ s^{-1} [*1(a).6*] and $k_{A'} = 7 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..73P066
7.16.2		*i*-octane	2.1×10^8 (est)		25	A′d–23	S = A′ = Rub. k estimated using $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*] and $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..74F341
7.16.3		hexa-decane	4.0×10^8 (est)		25	A′d–33	$^1O_2$* from microwave discharge, A′ = Rub. k estimated using $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*] and $k_{A'} = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl..74F341
7.17	1-cyclohexylamino 4-phenylamino-benzene 	EtOH	5.9×10^9		0	Od–23	S = MB, A′ = DMF. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*] and $k_{A'} = 5.3 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.29.12*].	Dall..72F518
7.17.1		EtOH	1.1×10^{10}		0	Od–20	S = MB, A′ = DMF. Measured ($k/k_{A'}$) = 47.4. k derived using $k_{A'}$ = *2.3×10^8 dm^3 mol^{-1} s^{-1} [*A3.15*].	Dall..72F518
7.18	1-cyclohexyl-amino-4-phenyl-aminobenzene hydrochloride 	EtOH	$< 1 \times 10^9$ (est)		0	Od–23	S = MB, A′ = DMF. No measurable effect.	Dall..72F518

TABLE 7. Rate constants for the interaction of singlet oxygen with aromatic amines — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
7.19	*N,N',N'',N'''*-tetramethyl-phenylene-diamine 	MeOH	5.6×10^8	1.77×10^{-4}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Mart72F519
7.19.1		MeOH	6.7×10^8	$(1.5 \pm 0.3) \times 10^{-4}$	rt	A'd-16	S = RB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].[a]	Youn....73E061
7.19.2		MeOH	$(1.0 \pm 0.2) \times 10^9$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit.	Youn...74F640
7.20	luminol 	D_2O (pD 11.8)	k_r = $(3 \pm 1) \times 10^7$ *1.8×10^7	β_r = $(1.7 \pm 0.6) \times 10^{-3}$	rt	A'd-35	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_d = 5 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math.76F662

[a] β has been corrected for contributions due to quenching of ^{3}S by substrate A.

TABLE 8. Rate constants for the interaction of singlet oxygen with amino acids and proteins

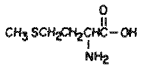
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
		[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]						
8.1	α–alanine 	D_2O (pD 8.1)	2.0×10^6 *1.2×10^6		22	A′d–22	$^1O_2$* directly from CW Nd–YAG laser (1065 nm), A′ = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math..75F147
8.1.1		H_2O/MeOH (1:1) v:v	$< 1 \times 10^7$		rt	A′d–5	S = MB, A′ = DPBF, ruby laser (694 nm).	Nils..72F516
8.2	methionine 	H_2O	2.2×10^7	2.0×10^{-2}	10	Od–15	S = MB. k derived using k_d = *4.4×10^5 s^{-1} [*1.1.3*]. The mechanism of oxidation is not clear.	Weil65F029
8.2.1		H_2O (pH 6)	8.4×10^7	5.2×10^{-2}	25	Ad–14	S = proflavin. β derived using $\phi_{ISC} = 0.73$. k derived using k_d = *4.4×10^5 s^{-1} [*1.1.3*].	Jori.70F732
8.2.2		H_2O (pH 7)	1.15×10^7 *5.06×10^6		rt	A′d–16	S = RB, A′ = DPF. Plots are nonlinear. Used slope as [A] → 0. k derived using $k_d = 1 \times 10^6$ (*4.4×10^5) s^{-1} [*1.1.3*].	Sysa.77F433
8.2.3		H_2O (pH 11)	$\leqslant 5.0 \times 10^7$ $\leqslant$ *2.2×10^7		rt	A′d–16	S = RB, A′ = DPF. Plots are nonlinear. Used slope as [A] → 0. k derived using $k_d = 1 \times 10^6$ (*4.4×10^5) s^{-1} [*1.1.3*].	Sysa..77F433
8.2.4		H_2O (pH 7.1)	8.6×10^6		25	Od–19	S = phenosafranine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
8.2.5		D_2O (pD 8.1)	3×10^7 *2×10^7		22	A′d–22	$^1O_2$* directly from CW Nd–YAG laser (1065 nm), A′ = bilirubin. k derived using $k_d = 5 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.2.6		D_2O (pD 7)	3.3×10^7		rt	A′d–16	S = RB, A′ = DPF. Plots are nonlinear. Used slope as [A] → 0. k derived using k_d(unreported).	Sysa..77F433
8.2.7		D_2O (pD 11)	1.57×10^7		rt	A′d–16	S = RB, A′ = DPF. Plots are nonlinear. Used slope as [A] → 0. k derived using k_d(unreported).	Sysa.77F433
8.2.8		H_2O/MeOH (1:1) v:v	3×10^7		rt	A′d–5	S = MB, A′ = DPBF, ruby laser (694 nm).	Nils..72F516

TABLE 8. Rate constants for the interaction of singlet oxygen with amino acids and proteins — Continued

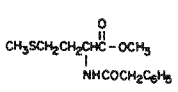
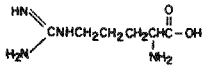
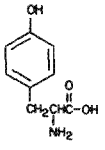
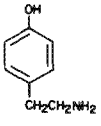
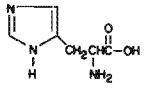
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
8.2.9		H_2O/MeOH (1:1) v:v	$k_r = 5\times10^6$		rt	Ad-17 A'd	S = MB, A' = DPBF. k_r measured relative to $k_r^{A'} = k_{A'}(MeOH) = 8 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.36.9*]. k_r derived using $k_d = 2.9 \times 10^5$ s^{-1} [*1.38*], $k_{Td}^A = 3 \times 10^8$ dm^3 mol^{-1} s^{-1}, and $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*8.2.8*].	Nils..72F516
8.3	CBZ-L-methionine methyl ester 	$CHCl_3$	$(1.4 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
8.4	arginine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$ (est)		25	Od-19	S = phenosafranine. No measurable effect.	Kral.78A360
8.5	tyrosine 	H_2O	2.7×10^7	1.66×10^{-2}	10	Od-15	S = MB. k derived using k_d = *4.4 $\times 10^5$ s^{-1} [*1.1.3*]. The mechanism of oxidation is not clear.	Weil65F029
8.6	tyramine 	H_2O (pH 10)	$(2.8 \pm 0.5) \times 10^8$ $k_r = 2.4 \times 10^8$		25	Ad-?	S = MB, A' = NaN_3. k and k_r by computer fit of rate parameters to experimental Φ versus [A] data.	Seel77F489
8.7	histidine 	H_2O	1.5×10^8	2.9×10^{-3}	rt	Od-14	S = proflavin. k derived using k_d = *4.4 $\times 10^5$ s^{-1} [*1.1.3*].	Sluy61F008
8.7.1		H_2O	5.43×10^9	9.2×10^{-5}	25	Ad-15	S = MB. k derived using k_d = 5.0×10^5 s^{-1} [*1.1*].	Usui..78F061
8.7.2		H_2O	1.3×10^8	3.44×10^{-3}	10	Od-15	S = MB. k derived using k_d = *4.4 $\times 10^5$ s^{-1} [*1.1.3*]. The mechanism of oxidation is not clear.	Weil65F029
8.7.3		H_2O (pH 7.1)	3.2×10^7		25	Od-19	S = phenosafraine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
8.7.4		D_2O (pD 8.1)	1.7×10^8 *1.1×10^8		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147

TABLE 8. Rate constants for the interaction of singlet oxygen with amino acids and proteins — Continued

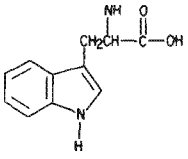
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
8.7.5		H_2O/MeOH (1:1) v:v	5×10^7		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Nils..72F516
8.7.6		H_2O/MeOH (1:1) v:v	$k_r = 7\times10^6$		rt	Ad-17 A'd	S = MB, A' = DPBF. k_r measured relative to $k_r^{A'} = k_{A'}$(MeOH) = 8×10^8 dm^3 mol^{-1} s^{-1} [*5.36.9*]. k_r derived using $k_d = 2.9 \times 10^5$ s^{-1} [*1.38*], k_{Td}^A = 1×10^6 dm^3 mol^{-1} s^{-1}, and $k_A = 5 \times 10^7$ dm^3 mol^{-1} s^{-1} [*8.7.5*].	Nils..72F516
8.8	tryptophan 	H_2O	2.5×10^8	1.78×10^{-3}	10	Od-15	S = MB. k derived using k_d = *4.4 $\times 10^5$ s^{-1} [*1.1.3*]. The mechanism of oxidation is not clear.	Weil65F029
8.8.1		D_2O (pD 8.1)	9×10^7 *5.9 $\times 10^7$		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_d = 5.0×10^4 (*3.1 $\times 10^4$) s^{-1} [*1.2.3*].	Math...75F147
8.8.2		MeOH	$(6.0 \pm 2.0) \times 10^6$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Smit78A338
8.8.3		EtOH	$\leqslant 5.0 \times 10^6$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Smit78A338
8.8.4		*N*-methyl-formamide	$(1.3 \pm 0.1) \times 10^8$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Smit78A338
8.8.5		H_2O/MeOH (1:1) Mole %	$(3.0 \pm 0.1)\times10^7$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Smit78A338
8.8.6		H_2O/MeOH (1:1) v:v	4×10^7		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Nils..72F516
8.8.7		H_2O/MeOH (1:1) v:v	$k_r = 4\times10^6$		rt	Ad-17 A'd	S = MB, A' = DPBF. k_r measured relative to $k_r^{A'} = k_{A'}$(MeOH) = 8×10^8 dm^3 mol^{-1} s^{-1} [*5.36.9*]. k_r derived using $k_d = 2.9 \times 10^5$ s^{-1} [*1.38*], k_{Td}^A = 2.0×10^9 dm^3 mol^{-1} s^{-1}, and $k_A = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} [*8.8.6*].	Nils..72F516
8.9	superoxide dismutase	D_2O (pD 8.1)	2.6×10^9 *1.6 $\times 10^9$		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_d = 5.0×10^4 (*3.1 $\times 10^4$) s^{-1} [*1.2.3*].	Math...75F147
8.9.1		D_2O (pD 8.1)	8.2×10^8 *5.1 $\times 10^9$		22	A'd-22	S = MB, A' = bilirubin. k derived using k_d = 5.0×10^4 (*3.1 $\times 10^4$) s^{-1} [*1.2.3*].	Math...75F147

TABLE 8. Rate constants for the interaction of singlet oxygen with amino acids and proteins — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
8.10	apo-superoxide dismutase	D_2O (pD 8.1)	2.5×10^9 *1.6×10^9		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.10.1		D_2O (pD 8.1)	1.1×10^9 *6.8×10^8		22	A'd-22	S = MB, A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.11	carbonic anhydrase	D_2O (pD 8.1)	8.0×10^8 *5.0×10^8		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.11.1		D_2O (pD 8.1)	6.5×10^8 *4.0×10^8		22	A'd-22	S = MB, A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.12	lysozyme	H_2O (pH 5.9)	$k_q = 3.5 \times 10^8$ $k_r = 1.6 \times 10^7$		20	Ad-14	S = acridine orange. k_q and k_r derived using $k_d = 5 \times 10^5$ s^{-1} [*1.1*].	Schm.72R087
8.12.1		H_2O	$k_r = 1.3 \times 10^8$		rt	Ad-28	S = eosin-Y. k_r derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Kepk.73R045
8.12.2		H_2O (pH 5.9)	$k_q = 4.1 \times 10^8$ $k_r = 2.9 \times 10^7$		20	Ad-14 28	S = acridine orange. k_q and k_r derived s^{-1} [*1.1*].	Schm.76F105
8.12.3		D_2O (pD 5.9)	$k_q = 3.3 \times 10^8$ $k_r = 1.5 \times 10^7$		20	Ad-14	S = acridine orange. k_q and k_r derived using k_d = *3.1×10^4 s^{-1} [*1.2.3*].	Schm.72R087
8.12.4		D_2O	$k_r = 2.5 \times 10^8$ *1.6×10^8		rt	Ad-28	S = eosin-Y. k_r derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Kepk.73R045
8.12.5		D_2O (pD 8.1)	1.5×10^9 *9.3×10^8		22	A'd-22	$^1O_2$* directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Math...75F147
8.12.6		D_2O	7.8×10^8	4.0×10^{-5}	18	Ad-15	S = 8-methoxypsoralen. k derived using k_d = *3.1×10^4 s^{-1} [*1.2.3*].	Popp.75F485
8.12.7		D_2O (pD 5.9)	$k_q = 5.9 \times 10^8$ *3.7×10^8 $k_r = 4.7 \times 10^7$ *2.9×10^7		20	Ad-14 28	S = acridine orange. k_q and k_r derived using $k_d = 5.0 \times 10^4$ (*3.1×10^4) s^{-1} [*1.2.3*].	Schm.76F105
8.13	trypsin	H_2O (pH 8.0)	7.1×10^9	7.0×10^{-5}	15	Pa-15	S = MB and FMN. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. β calculated from data reported in [66F197].	Stev73F659

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes

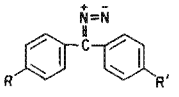
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
	[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]							
			COMPOUNDS 9.1 - 9.5 : 					
9.1	diazodiphenyl-methane (DDM)	MeOH	6.7×10^8 *4.8×10^8	$(2.1 \pm 0.4) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*]. Error is a 95% confidence limit.	Beth.77F113
9.1.1		$CHCl_3$	8.3×10^8 *5.0×10^8	$(2.0 \pm 0.4) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 1.67 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*]. Error is a 95% confidence limit.	Beth.77F113
9.1.2		$CHCl_3$	$k_r = 1.1 \times 10^9$ *5.7×10^8		rt	Ad-17 A'd	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = DMA. Measured ($k_r/k_r^{A'}$) = 12.2. k_r derived using $k_r^{A'} = 9.3 \times 10^7$ (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113
9.1.3		CH_3CN	1.1×10^9 *8.7×10^8	$(2.9 \pm 0.5) \times 10^{-5}$	rt	Ad-15	S =MB. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*]. Error is a 95% confidence limit.	Beth.77F113
9.1.4		CH_3CN	$k_r = 1.4 \times 10^9$ *3.8×10^8		rt	Ad-17 A'd	S = MB, A' = DMA. Measured ($k_r/k_r^{A'}$) = 8.0. k_r derived using $k_r^{A'} = 1.7 \times 10^8$ (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113
9.1.5		CH_3CN	$k_r = 2.4 \times 10^9$ *6.5×10^8		rt	Ad-17 A'd	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = DMA. Measured ($k_r/k_r^{A'}$) = 13.9. k_r derived using $k_r^{A'} = 1.7 \times 10^8$ (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113
			For more relative rates see		9.2-4, 9.4.3, 9.5, 9.5.1.			
9.2	diazo(4-bromo-phenyl)phenyl-methane [R = -Br]	CH_3CN	$k_r = 9.1 \times 10^8$ *3.8×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = $(6.48 \pm 0.32) \times 10^{-1}$. k_r derived using $k_r^{A'} = 1.4 \times 10^9$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113
9.3	diazo(4-methoxy-phenyl)phenyl-methane [R = -OMe]	CH_3CN	$k_r = 2.0 \times 10^9$ *8.5×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = 1.44 ± 0.07. k_r derived using $k_r^{A'} = 1.4 \times 10^9$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113
9.4	diazodi(4-chloro-phenyl)methane [R = R' = -Cl]	MeOH	$k_r = 3.8 \times 10^8$ *3.4×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = 0.577 ± 0.038. k_r derived using $k_r^{A'} = k_{A'} = 6.7 \times 10^8$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

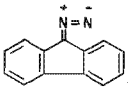
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.4.1		CH_3CN	6.6×10^8 *5.1×10^8	$(5.0 \pm 1.1) \times 10^{-5}$	rt	Ad-15	S = MB. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*]. Error is a 95% confidence limit.	Beth.77F113
9.4.2		CH_3CN	$k_r = 7.3 \times 10^8$ *2.0×10^8		rt	Ad-17 A'd	S = MB, A' = DMA. Measured ($k_r/k_r^{A'}$) = 4.29. k_r derived using $k_r^{A'} = 1.7 \times 10^8$ (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113
9.4.3		CH_3CN	$k_r = 7.5 \times 10^8$ *3.2×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = 0.537 ± 0.027. k_r derived using $k_r^{A'} = 1.4 \times 10^9$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113
9.5	diazodi(4-methyl-phenyl)methane [R = R' = -Me]	MeOH	$k_r = 9.4 \times 10^8$ *8.3×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = 1.41 ± 0.09. k_r derived using $k_{A'} = 6.7 \times 10^8$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113
9.5.1		CH_3CN	$k_r = 2.3 \times 10^9$ *9.7×10^8		rt	Ad-17 A'd	S = MB, A' = DDM. Measured ($k_r/k_r^{A'}$) = 1.65 ± 0.08. k_r derived using $k_r^{A'} = 1.4 \times 10^9$ (*5.9×10^8) dm^3 mol^{-1} s^{-1} [*A3.18*].	Beth.77F113
9.6	9-diazofluorene 	MeOH	3.3×10^8 *2.4×10^8	$(4.2 \pm 0.7) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*]. Error is a 95% confidence limit.	Beth.77F113
9.6.1		$CHCl_3$	5.1×10^7 *3.0×10^7	$(3.3 \pm 0.7) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using k_d = 1.67×10^4 (*1.0×10^4) s^{-1} [*1.5*]. Error is a 95% confidence limit.	Beth.77F113
9.6.2		$CHCl_3$	$k_r = 6.8 \times 10^7$ *3.5×10^7		rt	Ad-17 A'd	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = DMA. Measured ($k_r/k_r^{A'}$) = 0.735. k_r derived using $k_r^{A'}$ = 9.3×10^7 (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113
9.6.3		CH_3CN	1.0×10^8 *7.7×10^7	$(3.3 \pm 0.6) \times 10^{-4}$	rt	Ad-15	S = MB. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*]. Error is a 95% confidence limit.	Beth.77F113
9.6.4		CH_3CN	$k_r = 1.0 \times 10^8$ *2.7×10^7		rt	Ad-17 A'd	S = MB, A' = DMA. Measured ($k_r/k_r^{A'}$) = 0.587. k_r derived using $k_r^{A'}$ = 1.7×10^8 (*4.7×10^7) dm^3 mol^{-1} s^{-1} [*A3.10*].	Beth.77F113

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

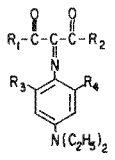
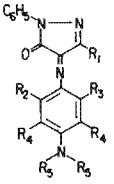
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
			COMPOUNDS 9.7 – 9.15 : 					
9.7	R_1 = t-Bu R_2 = t-Bu R_3 = H R_4 = Et	C_5H_5N	$\approx 1.6 \times 10^7$ $\approx$ *3.0×10^7 (est)		rt	Od-20	a	Smit..75F166
9.8	R_1 = Ph R_2 = Ph R_3 = H R_4 = Et	C_5H_5N	$\approx 1.6 \times 10^7$ $\approx$ *3.0×10^7 (est)		rt	Od-20	a	Smit..75F166
9.9	R_1 = -NHPh R_2 = -NHPh R_3 = H R_4 = Et	C_5H_5N	$\approx 1.6 \times 10^7$ $\approx$ *3.0×10^7 (est)		rt	Od-20	a	Smit..75F166
9.10[b]	R_1 = t-Bu R_2 = -NHPh R_3 = H R_4 = H	C_5H_5N	7.9×10^6 *1.5×10^7		rt	Od-20	a	Smit..75F166
9.11[b]	R_1 = t-Bu R_2 = -NHPh R_3 = H R_4 = Me	C_5H_5N	2.5×10^6 *4.8×10^7		rt	Od-20	a	Smit..75F166
9.12[b]	R_1 = Ph R_2 = -NHPh R_3 = H R_4 = H	C_5H_5N	4.0×10^6 *7.6×10^6		rt	Od-20	a	Smit..75F166
9.13[b]	R_1 = Ph R_2 = -NHPh R_3 = H R_4 = Me	C_5H_5N	7.9×10^6 *1.5×10^7		rt	Od-20	a	Smit..75F166
9.14[b]	R_1 = Ph R_2 = -NHPh R_3 = Me R_4 = Me	C_5H_5N	6.3×10^7 *1.2×10^8		rt	Od-20	a	Smit..75F166
9.15	R_1 = -NHPh R_2 = -NHPh R_3 = H R_4 = H	C_5H_5N	1.6×10^7 *3.0×10^7		rt	Od-20	a	Smit..75F166
			COMPOUNDS 9.16 – 9.27 : 					
9.16	R_1 = Me R_2 = H R_3 = H R_4 = H R_5 = H	CH_3CN	5.0×10^7 *4.0×10^7		rt	Od-20	c	Smit..75F166

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.17	R_1 = Me R_2 = Me R_3 = Me R_4 = Me R_5 = H	CH_3CN	5.0×10^8 *4.0×10^8		rt	Od-20	c	Smit..75F166
9.18	R_1 = Me R_2 = H R_3 = H R_4 = H R_5 = Me	C_5H_5N	4.0×10^7 *7.6×10^7		rt	Od-20	a	Smit..75F166
9.19	R_1 = Me R_2 = H R_3 = H R_4 = Me R_5 = Me	CH_3CN	6.3×10^6 *5.0×10^6		rt	Od-20	c	Smit..75F166
9.20	R_1 = Me R_2 = Me R_3 = Me R_4 = Me R_5 = Me	CH_3CN	4.0×10^6 *3.2×10^6		rt	Od-20	c	Smit..75F166
9.21	R_1 = Me R_2 = H R_3 = H R_4 = H R_5 = Et	CH_3CN	4.0×10^8 *3.2×10^8		rt	Od-20	c	Smit..75F166
9.21.1		C_5H_5N	4.0×10^7 *7.6×10^7		rt	Od-20	a	Smit..75F166
9.21.2		C_6H_6	1.2×10^7		rt	Od-20	e	Smit..75F166
9.22[b]	R_1 = Me R_2 = H R_3 = Me R_4 = H R_5 = Et	C_5H_5N	4.0×10^7 *7.6×10^7		rt	Od-20	a	Smit..75F166
9.23[b]	R_1 = Me R_2 = Me R_3 = Me R_4 = H R_5 = Et	CH_3CN	4.0×10^9 *3.2×10^9		rt	Od-20	c	Smit..75F166
9.23.1		C_5H_5N	6.3×10^8 *1.2×10^9		rt	Od-20	a	Smit..75F166
9.23.2		C_6H_6	1.1×10^9		rt	Od-20	e	Smit..75F166
9.24[b]	R_1 = t-Bu R_2 = H R_3 = Me R_4 = H R_5 = Et	CH_3CN	1.3×10^9 *1.0×10^9		rt	Od-20	c	Smit..75F166
9.24.1		C_5H_5N	1.65×10^8 *3.1×10^8		rt	Od-20	a	Smit..75F166
9.24.2		C_6H_6	1.3×10^8		rt	Od-20	e	Smit..75F166
9.25[b]	R_1 = t-Bu R_2 = Me R_3 = Me R_4 = H R_5 = Et	C_5H_5N	1.0×10^9 *1.9×10^9		rt	Od-20	a	Smit..75F166
9.26	R_1 = -NHCOPh R_2 = Me R_3 = Me R_4 = H R_5 = Et	C_5H_5N	1.0×10^9 *1.9×10^9		rt	Od-20	a	Smit..75F166

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — *Continued*

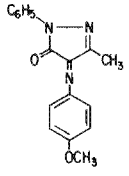
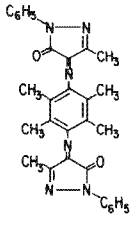
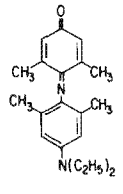
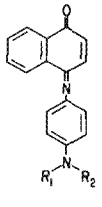
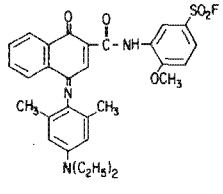
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.27	R_1 = Me R_2 = H R_3 = H R_4 = H R_5 = Ph	C_5H_5N	5.0×10^7 *9.5×10^7		rt	Od-20	a	Smit..75F166
9.28		CH_3CN	(not measurable)		rt	Od-20	S = RB, A′ = 2M2P. No measurable effect.	Smit..75F166
9.28.1		C_5H_5N	(not measurable)		rt	Od-20	S = RB, A′ = 2M2P. No measurable effect.	Smit..75F166
9.29		CH_3CN	(not measurable)		rt	Od-20	S = RB, A′ = 2M2P. No measurable effect.	Smit..75F166
9.29.1		C_5H_5N	(not measurable)		rt	Od-20	S = MB, A′ = 2M2P. No measurable effect.	Smit..75F166
9.30[b]		C_5H_5N	1.0×10^9 *1.9×10^9		rt	Od-20	a	Smit..75F166
	COMPOUNDS 9.31 - 9.32 : 							
9.31	R_1 = H R_2 = -Ph	C_5H_5N	$\leqslant 4.0 \times 10^7$ $\leqslant$ *7.6×10^7		rt	Od-20	a	Smit..75F166
9.32	R_1 = -Ph R_2 = -Ph	C_5H_5N	$\leqslant 3.2 \times 10^6$ $\leqslant$ *6.1×10^6		rt	Od-20	a	Smit..75F166
9.33		CH_3CN	3.9×10^{10} *3.1×10^{10}		rt	Od-20	a	Smit..75F166

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

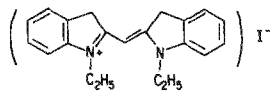
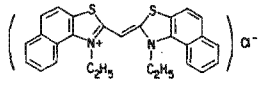
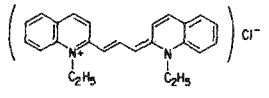
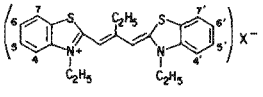
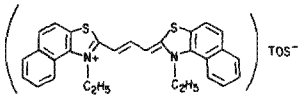
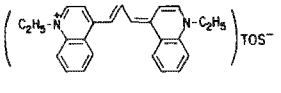
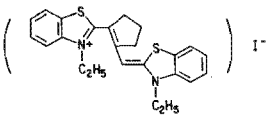
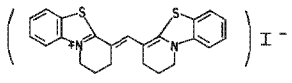
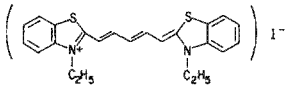
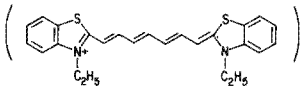
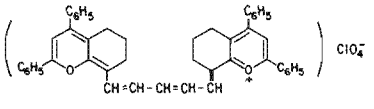
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.33.1		C_5H_5N	1.35×10^9 $*2.6 \times 10^9$		rt	Od-20	a	Smit..75F166
9.33.2		C_6H_6	4.7×10^9		rt	Od-20	e	Smit..75F166
9.34		MeOH	$k_r \approx 4.0 \times 10^5$ $*2.1 \times 10^5$		rt	Ad-15	d	Byer..76F071
9.35		MeOH	$k_r = 4.0 \times 10^5$ $\approx *2.1 \times 10^5$		rt	Ad-15	d	Byer..76F071
9.36		MeOH	$k_r = 3.4 \times 10^7$ $*1.8 \times 10^7$		rt	Ad-15	d	Byer..76F071
	COMPOUNDS 9.37 – 9.39 : 							
9.37	X = TOS^-	MeOH	$k_r = 3.5 \times 10^6$ $*1.8 \times 10^6$		rt	Ad-15	d	Byer..76F071
9.38	X = TOS^- $R_5 = R_{5'} = -OMe$	MeOH	$k_r = 6.7 \times 10^6$ $*3.5 \times 10^6$		rt	Ad-15	d	Byer..76F071
9.39	X = Br^- $R_5 = R_{5'} = -Cl$	MeOH	$k_r = 1.3 \times 10^6$ $*6.8 \times 10^5$		rt	Ad-15	d	Byer..76F071
9.40		MeOH	$k_r = 1.6 \times 10^7$ $*8.4 \times 10^6$		rt	Ad-15	d	Byer..76F071
9.41		MeOH	$k_r = 1.1 \times 10^8$ $*5.8 \times 10^7$		rt	Ad-15	S = 2-acetonaphthone, RB,Py, and fluorenone. k derived using $\Phi(^1O_2{}^*$ production) for each S and $k_d = 1.9 \times 10^5$ ($*1.0 \times 10^5$) s^{-1} [*1.3.1*]. k_r is an average for the 4 sensitizers.	Byer..76F071

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.41.1		CD_3OD	$k_r = 1.6 \times 10^8$ (est)		rt	Ad-15	S = 2-acetonaphthone. k estimated using $\Phi(^1O_2{}^*$ production) = 0.75 and $k_d = 1.3 \times 10^4$ s^{-1} (calc).	Byer..76F071
				COMPOUNDS 9.42 - 9.45 :				
9.42	X = Br^-	MeOH	$k_r = 1.6 \times 10^7$ *8.4×10^6		rt	Ad-15	d	Byer..76F071
9.43	$R_5 = R_{5'}$ = -OMe X = TOS^-	MeOH	$k_r = 3.1 \times 10^7$ *1.6×10^7		rt	Ad-15	d	Byer..76F071
9.44	$R_5 = R_{5'}$ = -Cl X = Br^-	MeOH	$k_r = 7.1 \times 10^6$ *3.7×10^6		rt	Ad-15	d	Byer..76F071
9.45	$R_5 = R_{5'}$ = -CN X = BF_4^-	MeOH	$k_r = 3.3 \times 10^6$ *1.7×10^6		rt	Ad-15	d	Byer..76F071
9.46		MeOH	$k_r = 7.3 \times 10^7$ *3.8×10^7		rt	Ad-15	d	Byer..76F071
9.47		MeOH	$k_r = 2.9 \times 10^8$ *1.5×10^8		rt	Ad-15	d	Byer..76F071
9.48		MeOH	$k_r \leqslant 3.0 \times 10^4$ *1.6×10^4		rt	Ad-15	d	Byer..76F071
9.49		MeOH	$k_r = 1.2 \times 10^8$ *6.3×10^7		rt	Ad-15	d	Byer..76F071

TABLE 9. Rate constants for the interaction of singlet oxygen with diazo-compounds and dyes — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
9.50		MeOH	$k_r = 1.5 \times 10^8$ *7.8×10^7		rt	Ad-15	d	Byer..76F071
9.51		MeOH	$k_r = 2.7 \times 10^7$ *1.4×10^7		rt	Ad-15	d	Byer..76F071
9.52		MeOH	$k_r = 1.3 \times 10^7$ *6.8×10^6		rt	Ad-15	d	Byer..76F071
9.53		MeOH	$k_r = 5.1 \times 10^7$ *2.7×10^7		rt	Ad-15	d	Byer..76F071
9.54		CH_3CN	$(3.0 \pm 0.8) \times 10^{10}$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Merk.72F260

[a]S = RB, A' = 2-methyl-2-pentene. k derived using $\beta_{A\cdot} = 4.3 \times 10^{-2}$ mol dm^{-3} [*2.40.19*] $k_d = 3.1 \times 10^4$ (*5.9×10^4) s^{-1} [*1.29*]. No evidence of chemical reaction.

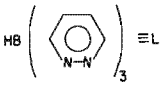
[b]The *N,N* dimethyl analog of these compounds showed a similar quenching efficiency to those reported, although a k value was not reported.

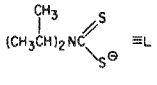
[c]S = RB, A' = 2-methyl-2-pentene. k derived using $\beta_{A\cdot} = 1.8 \times 10^{-2}$ mol dm^{-3} [*2.40.11*] and $k_d = 3.3 \times 10^4$ (*2.6×10^4) s^{-1} [*1.17*]. No evidence of chemical reaction.

[d]S = 2-acetonaphthone. k derived using $\Phi(^1O_2{}^*$ production) = 0.75 and $k_d = 1.9 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3.1*].

[e]S = azine, A' = 2-methyl-2-pentene. k derived using $\beta_{A\cdot} = 5.3 \times 10^{-2}$ mol dm^{-3} [*2.40.23*] and $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*]. No evidence of chemical reaction.

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.1	$NiCl_2 \cdot 6H_2O$	2-butoxy-ethanol	3.1×10^8 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using k_d = 3.8×10^5 s^{-1} [*1(a).4*] and k_A = 7×10^7 dm^3 mol^{-1} s^{-1}.	Carl...72F319
10.2	$CoCl_2 \cdot 6H_2O$	2-butoxy-ethanol	4.8×10^7 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using k_d = 3.8×10^5 s^{-1} [*1(a).4*] and k_A = 7×10^7 dm^3 mol^{-1} s^{-1}.	Carl...72F319
10.3	$MnCl_2 \cdot 6H_2O$	2-butoxy-ethanol	$< 1.0 \times 10^6$ (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using k_d = 3.8×10^5 s^{-1} [*1(a).4*] and k_A = 7×10^7 dm^3 mol^{-1} s^{-1}.	Carl...72F319
10.4	$MnCl_2 \cdot 4H_2O$	*i*-octane	$\leqslant 1.0 \times 10^6$ (est)	25	Ad-23	S = A = Rub. k estimated using k_A = 7.3×10^7 dm^3 mol^{-1} s^{-1}. and k_d = 4.7×10^4 s^{-1} [*1(a).6.1*].	Carl..74F341
10.5	Ni(II) bis[hydrotris-(1-pyrazoyl)-borate] 	$CHCl_3$	$(2.1 \pm 0.4) \times 10^6$	rt	Ad-33	S = A = Rub. k derived using k_A = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr.79A050
10.6	Ni(II) bis[isopropyl-xanthate] $[(CH_3)_2CHOCS_2]_2Ni$	*i*-octane	5.4×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using k_A = 7.3×10^7 dm^3 mol^{-1} s^{-1}. and k_d = 4.0×10^4 s^{-1}[*1(a).6*]	Carl.74F642
10.7	Ni(II) bis(*N*-phenyl-dithiocarbamate) $[C_6H_5NHCS_2]_2Ni$	$CHCl_3$	$(1.1 \pm 0.2) \times 10^{10}$	rt	Ad-33	S = A = Rub. k derived using k_A = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.67×10^4 s^{-1} [*1.5*].	Monr.79A050
10.8	Ni(II) bis(*N*,*N*-dimethyl-dithiocarbamate) $[(CH_3)_2NCS_2]_2Ni$	CH_2Cl_2	1.8×10^7	rt	A'd-19	S = A = Tetr. k derived using k_A = 3.0×10^7 dm^3 mol^{-1} s^{-1}. [*3.62*].	Byst.75F654
10.8.1		C_6H_6/EtOH (8:1) v:v	not measurable	22	Pa-13	S = RB, A = TMHP, P = nitroxy radicals.	Ivan....75F445
10.9	Ni(II) bis(*N*,*N*-diethyl-dithiocarbamate) $[(CH_3CH_2)_2NCS_2]_2Ni$	CCl_4/MeOH (98:2) v:v	$(6.6 \pm 0.6) \times 10^9$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238

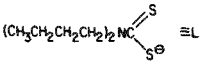
LIGANDS 10.10 - 10.15 : 

10.10	Mn(II) bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	$< 1.0 \times 10^7$ (est)	rt	Ad-23	S = A = Rub. k estimated using k_A = 7×10^7 dm^3 mol^{-1} s^{-1} and k_d = 7.3×10^3 s^{-1}.	Carl..73P066
10.11	Co(II) bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	1.9×10^9 (est)	rt	Ad-23	S = A = Rub. k estimated using k_A = 7×10^7 dm^3 mol^{-1} s^{-1} and k_d = 7.3×10^3 s^{-1}.	Carl..73P066
10.11.1		*i*-octane	1.9×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using k_A = 7.3×10^7 dm^3 mol^{-1} s^{-1}.	Carl..74F341
10.11.2		hexadecane	9.0×10^8 (est)	25	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. k estimated using k_A = 7.3×10^7 dm^3 mol^{-1} s^{-1} and k_d = 9.0×10^4 s^{-1} [*1(a).7*].	Carl..74F341
10.12	Ni(II) bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	3.4×10^9 (est)	rt	Ad-23	S = A = Rub. k estimated using k_A = 7×10^7 dm^3 mol^{-1} s^{-1} and k_d = 7.3×10^3 s^{-1}.	Carl..73P066
10.13	Cu(II)bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	$< 1.0 \times 10^7$ (est)	rt	Ad-23	S = A = Rub. k estimated using k_A = 7.3×10^7 dm^3 mol^{-1} s^{-1} and k_d = 7.3×10^3 s^{-1}.	Carl..73P066

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.14	Zn(II) bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	$< 1.0 \times 10^7$ (est)	rt	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl..73P066
10.15	Fe(III) bis(*N*,*N*-diiso-propyldithiocarbamate)	CH_2Cl_2	3.8×10^9 (est)	rt	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and	Carl..73P066
10.15.1		CH_2Cl_2	4.3×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl..74F341
10.15.2		CH_2Cl_2	3.9×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl.74F642
10.15.3		*i*-octane	3.8×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl.74F642
10.15.4		hexadecane	1.2×10^9 (est)	25	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl..74F341

LIGANDS 10.16 - 10.19 :



10.16	Co(II) bis(*N*,*N*-dibutyl-dithiocarbamate)	CCl_4/MeOH (98:2) v:v	$(1.2 \pm 0.2) \times 10^9$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238
10.17	Ni(II) bis(*N*,*N*-dibutyl-dithiocarbamate)	CH_2Cl_2	9.0×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 8 \times 10^3$ s^{-1}.	Carl..74F341
10.17.1		CH_2Cl_2	8.0×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl.74F642
10.17.2		CH_2Cl_2	5.7×10^9	rt	A'd-19	S = A = Tetr. k derived using $k_A = 3.0 \times 10^7$ dm^3 mol^{-1} s^{-1}. [*3.62*].	Byst.75F654
10.17.3		$CHCl_3$	$(8.1 \pm 1.3) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.17.4		C_6H_5Br	2.6×10^8 (est)	0	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. Measured $k/[(k_d/[A]) + k_A] = 2.0$ at $[A] = 1.5 \times 10^{-4}$ mol dm^{-3}. k estimated using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Guil.73F333
10.17.5		$C_6H_5CH_3$	4.3×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.17.6		*i*-octane	7.0×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl...72F319
10.17.7		*i*-octane	1.7×10^{10} (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*].	Carl..74F341
10.17.8		hexadecane	1.0×10^9 (est)	25	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl..74F341
10.17.9		hexadecane	9.0×10^8 (est)	25	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl...72F319

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

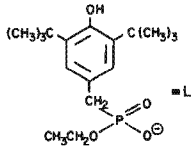
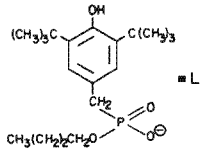
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.17.10		CCl_4/MeOH (98:2) v:v	$(4.1 \pm 0.6) \times 10^9$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238
10.17.11		CS_2/MeOH (98:2) v:v	$(4.0 \pm 1.5) \times 10^9$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Floo..73F334
10.17.12		C_6H_6/EtOH (8:1) v:v	1.6×10^9 (est)	22	Pa-13	S = RB, A = TMHP, P = Nitroxy radicals. k estimated using $k_d = 3 \times 10^4$ s^{-1} (calc).	Ivan....75F445
10.17.13		CH_2Cl_2/MeOH /C_5H_5N (94:3:3) v:v:v	$\leqslant 1.0 \times 10^9$ (est)	25	Ad-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}. Interference by chelate ozonide reaction to give colored products.	Carl...72F319
10.18	Cu(II) bis(*N,N*-dibutyl-dithiocarbamate)	CCl_4/MeOH (98:2) v:v	$< 5 \times 10^8$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238
10.19	*Zn(II)*bis(*N,N*-dibutyl-dithiocarbamate)	CS_2/MeOH (98:2) v:v	$(2.0 \pm 1.0) \times 10^7$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Floo..73F334
10.19.1		C_6H_5Br	$\leqslant 1 \times 10^6$ (est)	0	Ad-33	$^1O_2$* from microwave discharge, A′ = Rub. No measurable effect.	Guil.73F333
10.20	Ni(II)bis(*N,N*-di-phenyldithiocarbamate) $[(C_6H_5)_2NCS_2]_2Ni$	$CHCl_3$	$(6.3 \pm 1.0) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.20.1		*i*-octane	$< 1.0 \times 10^6$ (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*].	Carl..74F341
10.21	Ni(II) bis[*N*-(*p*-methyl phenyl)dithiocarbamate] $[(4\text{-}CH_3C_6H_4)NHCS_2]_2Ni$	$CHCl_3$	$(1.1 \pm 0.2) \times 10^{10}$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.22	Ni(II) bis[*O*-ethyl-3,5-di-*t*-butyl-4-hydroxy-benzylphosphonate]	CH_2Cl_2	6.0×10^6	rt	A′d-19	S = A = Tetr. k derived using $k_A = 3.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.62*].	Byst.75F654
10.22.1		$CHCl_3$	$(2.2 \pm 0.4) \times 10^7$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.23	Ni(II) bis[*O*-butyl-3,5-di-*t*-butyl-4-hydroxybenzyl-phosphonate]	CH_2Cl_2	1.4×10^7 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl...72F319
10.23.1		CH_2Cl_2	1.6×10^7 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl.74F642
10.23.2		C_6H_6	1.4×10^7	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.23.3		2-butoxy-ethanol	3.4×10^7 (est)	0	Ad-33	$^1O_2$ from microwave discharge, A = Rub. k estimated using $k_d = 3.8 \times 10^5$ s^{-1} [*1(a).4*] and $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl...72F319
10.23.4		C_6H_5Br	1.3×10^7 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. Measured $k/[(k_d/[A]) + k_A] = 0.1$ at $[A] = 1.5 \times 10^{-4}$ mol dm^{-3}. k estimated using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*]. Q exists as a trimer in solution.	Guil.73F333

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

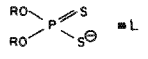
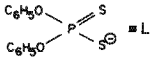
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.23.5		$C_6H_5CH_3$	2.0×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.23.6		$CCl_4/CHCl_3$ (9:1) v:v	9.0×10^6	rt	Ad–23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 5.2 \times 10^3$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
10.23.7		CH_2Cl_2/MeOH /C_5H_5N (94:3:3) v:v:v	1.0×10^7 (est)	25	Ad–32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl...72F319
		LIGANDS 10.24 AND 10.26 : 					
10.24	Ni(II) bis(*O,O'*-diethyl-dithiophosphate) [R = Et]	$CHCl_3$	$(9.5 \pm 1.5) \times 10^9$	rt	Ad–33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.25	Ni(II) bis[*O,O'*-diiso-propyldithio-phosphate] [R = *-i-*Pr]	CH_2Cl_2	5.4×10^9 (est)	rt	Ad–23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl..73P066
10.25.1		CCl_4/MeOH (98:2) v:v	$(7.6 \pm 1.0) \times 10^9$	rt	Ad–5	S = MB, A = DPBF, flash photolysis.	Furu.78E238
10.26	Co(II) bis[*O,O'*-dicyclo-hexyldithio-phosphate] [R = *-cyclo-*C_6H_{11}]	$C_6H_5CH_3$	2.7×10^9 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.27	Ni(II) bis(dicyclo-hexyldithio-phosphinate) [(*cyclo-*$C_6H_{11})_2PS_2]_2$Ni	$CHCl_3$	$(5.7 \pm 0.9) \times 10^9$	rt	Ad–33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
		LIGANDS 10.28 - 10.33 : 					
10.28	Co(II) bis(*O,O'*-di-phenyldithiophosphate)	C_6H_6	1.2×10^9	rt	Ad–23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.29	Ni(II) bis(*O,O'*-di-phenyldithiophosphate)	$CHCl_3$	$(1.1 \pm 0.2) \times 10^{10}$	rt	Ad–33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.29.1		C_6H_6	2.5×10^9	rt	Ad–23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.30	Cu(II) bis(*O,O'*-di-phenyldithiophosphate)	C_6H_6	1.7×10^6	rt	Ad–23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.31	Zn(II) bis(*O,O'*-di-phenyldithiophosphate)	C_6H_6	5.0×10^6	rt	Ad–23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.32	Cr(II) bis(*O,O'*-di-phenyldithiophosphate)	C_6H_6	3.2×10^6	rt	Ad–23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

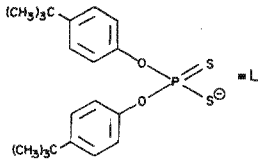
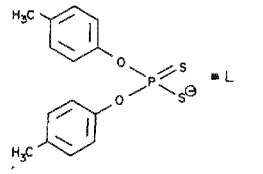
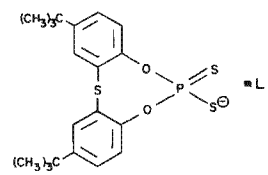
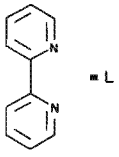
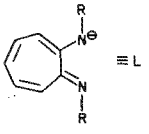
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.33	Pb(II) bis(*O,O'*-di-phenyldithiophosphate)	C_6H_6	3.4×10^7	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
			LIGANDS 10.34 - 10.36 :				
							
10.34	Co(II) bis(*O,O'*-di-*p-t*-butylphenyldithio-phosphate)	C_6H_6	1.2×10^9	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.35	Ni(II) bis(*O,O'*-di-*p-t*-butylphenyldithio-phosphate)	C_6H_6	2.3×10^9	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.36	Cu(II) bis(*O,O'*-di-*p-t*-butylphenyldithio-phosphate)	C_6H_6	7.0×10^6	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
			LIGANDS 10.37 - 10.39 :				
							
10.37	Co(II) bis(*O,O'*-di-4-methylphenyldithio-phosphate)	C_6H_6	1.1×10^9	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.38	Ni(II) bis(*O,O'*-di-4-methylphenyldithio-phosphate)	C_6H_6	2.3×10^9	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.39	Cu(II) bis(*O,O'*-di-4-methylphenyldithio-phosphate)	C_6H_6	2.0×10^6	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
			LIGANDS 10.40 -10.44 :				
							
10.40	Co(II) bis[2,2'-thiobis-(*O,O'*-di-*p-t*-butylphenyl)-dithiophosphate]	C_6H_6	8.7×10^8	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.41	Ni(II) bis[2,2'-thiobis-(*O,O'*-di-*p-t*-butylphenyl)-dithiophosphate]	C_6H_6	2.2×10^9	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.42	Zn(II) bis[2,2'-thiobis-(*O,O'*-di-*p-t*-butylphenyl)-dithiophosphate]	C_6H_6	4.35×10^6	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.43	Cd(II) bis[2,2'-thiobis-(*O,O'*-di-*p*-*t*-butylphenyl)-dithiophosphate]	C_6H_6	8.4×10^6	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.44	Pb(II) bis[2,2'-thiobis-(*O,O'*-di-*p*-*t*-butylphenyl)-dithiophosphate]	C_6H_6	1.0×10^7	rt	Ad-23	S = A = Rub. k derived using $k_A = 3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.8 \times 10^4$ s^{-1}.	Edil....78F497
10.45	tris(2,2'-bipyridine) Ru(II)·Cl_2	CCl_4/MeOH (98:2) v:v	$\leqslant 1.0 \times 10^9$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238

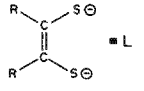


LIGANDS 10.46 – 10.47 :



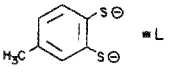
10.46	Ni(II) bis(1-methyl-amino-2-methylimino-cycloheptatriene) [R = -CH_3]	$CHCl_3$	$(6.1 \pm 1.0) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.47	Ni(II) bis[1-(4'-methyl-phenyl)amino-2-(4'-methylphenyl)imino-cycloheptatriene] [R = -4'-$CH_3C_6H_4$]	$CHCl_3$	$(5.6 \pm 0.9) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050

LIGANDS 10.48 AND 10.50 :



10.48	Ni(II) bis[dithio-biacetyl] [R = -Me]	$C_6H_5CH_3$	2.8×10^{10} (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.49	Ni(II) bis(dithio-hexafluorobiacetyl) [R = -CF_3]	$CHCl_3$	$(8.1 \pm 1.3) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.50	Ni(II) bis(dithio-benzil) [R = -Ph]	$CHCl_3$	$(1.1 \pm 0.2) \times 10^{10}$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.50.1		$C_6H_5CH_3$	2.2×10^{10} (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

LIGANDS 10.51 AND 10.52 :



10.51	Co(II) bis[μ-toluene-3,4-dithiolato]TBA_2	$C_6H_5CH_3$	3.5×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

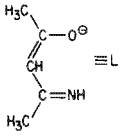
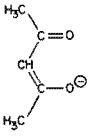
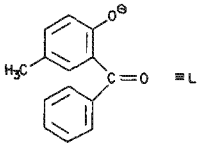
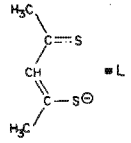
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.52	Ni(II) bis[μ-toluene-3,4-dithiolato]TBA$_2$	$C_6H_5CH_3$	5.8×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.53	Ni(II) bis[4-imino-2-pentene-2-ol] 	$C_6H_5CH_3$	7.2×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
			LIGANDS 10.54 - 10.62 : 				
10.54	Co(II) bis(acetylacetonate)	$C_6H_5CH_3$	1×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.54.1		$CCl_4/CHCl_3$ (9:1) v:v	1.46×10^8	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 8.2 \times 10^4$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
10.55	Ni(II) bis(acetylacetonate)	CH_2Cl_2	1.5×10^8 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 8 \times 10^3$ s^{-1}.	Carl..74F341
10.55.1		CH_2Cl_2	7.5×10^7 (est)	rt	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl..73P066
10.55.2		2-butoxyethanol	7.5×10^7 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_d = 3.8 \times 10^5$ s^{-1} [*1(a).4*] and $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Carl...72F319
10.55.3		C_6H_5Br	6.5×10^7 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. Measured $k/[(k_d/[A]) + k_A] = 0.5$ at [A] = 1.5×10^{-4} mol dm^{-3}. k estimated using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*]. Q exists as a trimer in solution.	Guil.73F333
10.55.4		$C_6H_5CH_3$	3×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.55.5		$CCl_4/CHCl_3$ (9:1) v:v	8.2×10^7	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 4.6 \times 10^4$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
10.56	Cu(II) bis(acetylacetonate)	$C_6H_5CH_3$	1×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.56.1		$CCl_4/CHCl_3$ (9:1) v:v	3.7×10^6	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 2.1 \times 10^3$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [1.8].	Hrdl...74F645
10.57	Zn(II) bis(acetyl-acetonate)	$CCl_4/CHCl_3$ (9:1) v:v	1.08×10^7	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 6.1 \times 10^3$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [1.8].	Hrdl...74F645
10.58	Cr(III) tris(acetyl-acetonate)	$CCl_4/CHCl_3$ (9:1) v:v	5.0×10^5	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 3.0 \times 10^2$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [1.8].	Hrdl...74F645
10.59	Mn(III) tris(acetyl-acetonate)	$C_6H_5CH_3$	5×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.60	Fe(III) tris(acetyl-acetonate)	$CCl_4/CHCl_3$ (9:1) v:v	8.7×10^7	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 4.9 \times 10^4$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [1.8].	Hrdl...74F645
10.61	Co(III) tris(acetyl-acetonate)	$CCl_4/CHCl_3$ (9:1) v:v	9.2×10^8	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 5.2 \times 10^5$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [1.8].	Hrdl...74F645
10.62	Ni(II) bis(acetyl-acetonate)-2H_2O	CCl_4/MeOH (98:2) v:v	$(6.6 \pm 0.6) \times 10^7$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Furu.78E238
10.63	Ni(II) bis[2-hydroxy-5-methylbenzophenone]	$C_6H_5CH_3$	3.9×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.64	Ni(II) bis[dithio-acetylacetonate]	C_6H_5Br	2.3×10^8	0	Ad-23	$^1O_2$* from microwave discharge, A = Rub. Measured $k/[(k_d/[A]) + k_A] = 1.8$ at [A] = 1.5×10^{-4} mol dm^{-3}. k derived using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [1.34].	Guil.73F333





LIGANDS 10.65 - 10.67 :

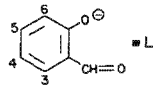


TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

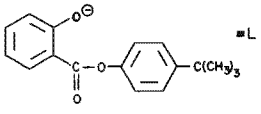
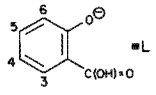
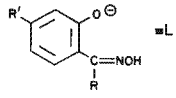
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.65	Ni(II) bis(salicyl-aldehyde)·2H_2O	$CHCl_3$	$(4.6 \pm 0.7) \times 10^7$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.66	Ni(II) bis(5-bromo-salicylaldehyde)·2H_2O [R_5 = -Br]	$CHCl_3$	$(5.3 \pm 0.8) \times 10^7$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.67	Ni(II) bis(5-methoxy-salicylaldehyde)·2H_2O [R_5 = -OCH_3]	$CHCl_3$	$(1.2 \pm 0.2) \times 10^8$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.68	Ni(II) bis[*p*-*t*-butylphenylsalicylate] 	CCl_4 /$CHCl_3$ (9:1) v:v	1.5×10^7	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 8.5 \times 10^3$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
			LIGANDS 10.69 - 10.70 : 				
10.69	Co(II) bis[3,5-diisopropyl-salicylate] [$R_3 = R_5$ = -*i*-Pr]	$C_6H_5CH_3$	3.0×10^7 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.70	Ni(II) bis[3,5-di-isopropylsalicylate] [$R_3 = R_5$ = -*i*-Pr]	$C_6H_5CH_3$	5.0×10^7 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
			LIGANDS 10.71 - 10.75 : 				
10.71	Ni(II) bis(salycil-aldehyde oxime)	$C_6H_5CH_3$	5.9×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.72	Ni(II) bis(2'-hydroxyaceto-phenone oxime) [R = -Me]	$C_6H_5CH_3$	5.2×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.73	Ni(II) bis[2'-hydroxy-4'-methyl-acetophenone oxime] [R = R' = -Me]	C_6H_6	$(3.0 \pm 0.3) \times 10^9$	25	Ad-8	S = An, A = DPBF, ruby laser (694 nm).	Farm.73F438
10.73.1		C_6H_6	$(3.1 \pm 0.3) \times 10^9$	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.74	Pd(II) bis [2'-hydroxy-4'-*t*-butyl-octadecanophenone oxime] [R = -heptadecyl, R' = -*t*-Bu]	C_6H_6	$(6.0 \pm 0.5) \times 10^7$	25	Ad-8	S = An, A = DPBF, ruby laser (694 nm).	Farm.73F438
10.75	Ni(II) bis[2'-hydroxy-4'-methyl-dodecanophenone oxime] [R = -undecyl, R' = -Me]	C_6H_6	$(2.7 \pm 0.3) \times 10^9$	25	Ad-8	S = An, A = DPBF, ruby laser (694 nm).	Farm.73F438

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

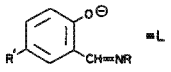
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.75.1		C_6H_6	$(2.8 \pm 0.3) \times 10^9$	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.75.2		$C_6H_5CH_3$	5.7×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
			LIGANDS 10.76 - 10.91 :				
			 =L				
10.76	Ni(II) bis[2-(form-imidoyl)phenol]	$CHCl_3$	$(3.2 \pm 0.5) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.77	Ni(II) bis[*o*-*N*-phenyl-aminoformimidoyl-phenol] [R = $-NHC_6H_5$]	$C_6H_5CH_3$	7.5×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.78	Ni(II) bis[2-(*N*-iso-propylformimi-doyl)phenol] [R = *-i*-Pr]	$CHCl_3$	$(2.6 \pm 0.4) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Mon.79A050
10.78.1		$C_6H_5CH_3$	5.9×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.79	Ni(II) bis[2-(*N*-butyl-formimidoyl) phenol] [R = -Bu]	$CHCl_3$	$(2.8 \pm 0.5) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.80	Ni(II) bis[2-(*N*-butyl-formimdoyl)-4-bromophenol] [R = -Bu, R′ = -Br]	$CHCl_3$	$(3.7 \pm 0.6) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.81	Ni(II) bis[2-(*N*-butyl-formimidoyl)-4-methoxy phenol] [R = -Bu, R′ = $-OCH_3$]	$CHCl_3$	$(3.4 \pm 0.6) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.81.1		CH_2Cl_2	$\geqslant 1.0 \times 10^9$ (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 7.3 \times 10^3$ s^{-1}.	Carl...72F319
10.81.2		CH_2Cl_2	2.0×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 8 \times 10^3$ s^{-1}.	Carl..74F341
10.81.3		*i*-octane	2.6×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*].	Carl..74F341
10.81.4		*i*-octane	2.4×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl.74F642
10.81.5		*i*-octane	2.4×10^9 (est)	rt	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl..73P066
10.81.6		*i*-octane	4.0×10^9 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl.74F642

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.81.7		hexadecane	2.0×10^8 (est)	25	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl...72F319
10.81.8		hexadecane	4.0×10^8 (est)	25	Ad-33	$^1O_2$* from a microwave discharge, A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl..74F341
10.81.9		*i*-octane/ MeOH/ C_5H_5N (94:3:3) v:v:v	3.5×10^9 (est)	25	Ad-32	$^1O_2$* from $(PhO)_3PO_3$ decomp, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 5.0 \times 10^4$ s^{-1}.	Carl..72F319
10.82	Ni(II) bis[*o*-(*N*-*sec*-butylformimidoyl)-phenol] [R = -*sec*-Bu]	$C_6H_5CH_3$	4.0×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.83	Ni(II) bis[*o*-(*N*-*t*-butylformimidoyl)-phenol] [R = -*t*-Bu]	C_6H_6	$(2.6 \pm 0.2) \times 10^8$	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.84	Ni(II) bis[*o*-(*N*-cyclohexylformimidoyl)-phenol] [R = -*cyclo*-C_6H_{11}]	$C_6H_5CH_3$	4.7×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.85	Co(II) bis[*o*-(*N*-phenylformimidoyl) phenol] [R = -Ph]	$C_6H_5CH_3$	3.2×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.86	Ni(II) bis[*o*-(*N*-phenylformimidoyl)-phenol] [R = -Ph]	$C_6H_5CH_3$	7.8×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.87	Cu(II) bis[*o*-(*N*-phenylformimidoyl)-phenol] [R = -Ph]	$C_6H_5CH_3$	4.0×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.88	Co(II) bis[*o*-(*N*-dodecylformimidoyl)-phenol] [R = -*n*-dodecyl]	$C_6H_5CH_3$	2.4×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.89	Ni(II) bis[*o*-(*N*-dodecylformimidoyl)-phenol] [R = -*n*-dodecyl]	$C_6H_5CH_3$	7.0×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.90	Cu(II) bis[*o*-(*N*-dodecylformimidoyl)-phenol] [R = -*n*-dodecyl]	$C_6H_5CH_3$	5.0×10^7 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.91	Ni(II)bis[*o*-(*N*-(*p*-anilinophenyl)-formimidoyl)phenol] [R = -$C_6H_4NHC_6H_5$]	$C_6H_5CH_3$	1.7×10^9 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

LIGANDS 10.92 - 10.97 :

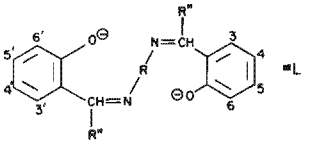
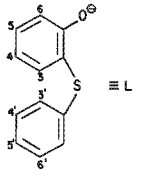


TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.92	Co(II) 2,2′-[ethylenebis(nitrilomethylidyne)] diphenol [R = $-CH_2CH_2-$, R″ = –H]	$C_6H_5CH_3$	1.0×10^{10} (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.93	Ni(II) 2,2′-[ethylenebis(nitrilomethylidyne)] diphenol [R = $-CH_2CH_2-$, R″ = –H]	$C_6H_5CH_3$	5.3×10^9 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.94	Ni(II) 2,2′-[ethylenebis(nitriloethylidyne)] diphenol [R = $-CH_2CH_2-$, R″ = $-CH_3$]	$C_6H_5CH_3$	3.4×10^9 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.95	Ni(II) 2,2′-[ethylenebis(nitrilodecylidyne)] di-*p*-cresol [R = $-CH_2CH_2-$, R″ = n-C_9H_{19}]	$C_6H_5CH_3$	4.8×10^9 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.96	Ni(II) 2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenol [R = $-C_6H_4-$, R″ = –H]	$C_6H_5CH_3$	3.7×10^9 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.97	Ni(II) 2,2′-[1,8-naphthylenebis(nitrilomethylidyne)]diphenol [R = $-C_{10}H_6-$, R″ = –H]	$C_6H_5CH_3$	1.2×10^{10} (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

LIGANDS 10.98 – 10.114 :



10.98	Ni(II) aquo[2,2′-thiobis(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	1.4×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.99	Ni(II) aquo[2,2′-thiobis(3,4-dimethyl)phenolate] [$R_3 = R_4$ = –Me]	$C_6H_5CH_3$	1.2×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.100	Ni(II) ammine[2,2′-thiobis(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	4.8×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.101	Ni(II) ethylamine [2,2′-thiobis(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	3.1×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.102	Ni(II) ethylamine [2,2′-thiobis(3,4-dimethyl)phenolate] [$R_3 = R_4$ = –Me]	$C_6H_5CH_3$	4.1×10^8 (est)	rt	Ad–25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063

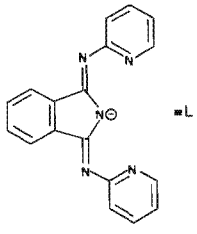
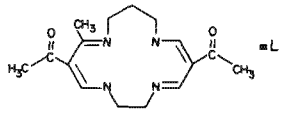
TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.103	Ni(II) propylamine [2,2′-thiobis(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	3.0×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.104	Co(II) *n*-butylamine[2,2′-thiobis-(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	3.7×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.105	Ni(II) butylamine [2,2′-thiobis(4-it-octyl)phenolate] [R_4 = -*t*-octyl]	$CHCl_3$	$(1.7 \pm 0.3) \times 10^8$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.105.1		C_6H_6	$(1.1 \pm 0.1) \times 10^8$	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.105.2		C_5H_5Br	1.3×10^8	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. Measured $k_Q/[(k_d/[A]) + k_A] = 1.0$ at $[A] = 1.5 \times 10^{-4}$ mol dm^{-3}. k derived using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*]. Q exists as a tetramer in solution.	Guil.73F333
10.105.3		2-butoxy-ethanol	2.8×10^8 (est)	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 3.8 \times 10^5$ s^{-1} [*1(a).4*].	Carl...72F319
10.105.4		$C_6H_5CH_3$	4.0×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.105.5		*i*-octane	1.8×10^8 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl...72F319
10.105.6		*i*-octane	2.0×10^8 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*].	Carl..74F341
10.105.7		*i*-octane	1.4×10^8 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl.74F642
10.105.8		hexadecane	8.0×10^7 (est)	25	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl...72F319
10.105.9		hexadecane	1.0×10^8 (est)	25	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl..74F341
10.105.10		CCl_4 /$CHCl_3$ (9:1) v:v	1.08×10^8	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 6.1 \times 10^4$ dm^3 mol^{-1} at $[A] = 5 \times 10^{-6}$ mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645
10.105.11		CS_2/MeOH (98:2) v:v	$(1.5 \pm 0.8) \times 10^8$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Floo..73F334
10.105.12		*i*-octane/ MeOH/C_5H_5N (94:3:3) v:v:v	2.7×10^8 (est)	25	Ad-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 5.0 \times 10^4$ s^{-1}.	Carl..72F319

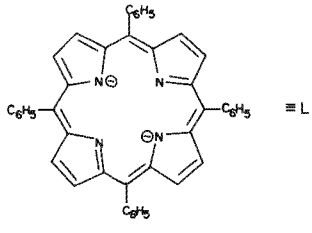
TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.106	Ni(II) butyl-amine[2,2′-thiobis-(3,4-dimethyl)phenolate] [R_3 = R_4 = -Me]	$C_6H_5CH_3$	2.5×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.107	Ni(II) cyclohexyl-amine[2,2′-thiobis-(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	1.8×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.108	Ni(II) cyclo-hexylamine[2,2′-thiobis-(3,4-dimethyl)phenolate] [R_3 = R_4 = -Me]	$C_6H_5CH_3$	3.4×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.109	Ni(II) aniline[2,2′-thiobis(4-*t*-octyl)-phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	1.9×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.110	Ni(II) dodecyl-amine[2,2′-thiobis-(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	2.6×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.111	Ni(II) dodecylamine [2,2′-thiobis-(3,4-dimethyl)phenolate] [R_3 = R_4 = -Me]	$C_6H_5CH_3$	3.9×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.112	Ni(II) didodecyl-amine[2,2′-thiobis-3,4-dimethyl)phenolate] [R_3 = R_4 = -Me]	$C_6H_5CH_3$	3.2×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.113	Ni(II) triethanol-amine[2,2′-thiobis-(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	$C_6H_5CH_3$	1.1×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.114	Ni(II) bis[2,2′-thiobis-(4-*t*-octyl)phenolate] [R_4 = -*t*-octyl]	C_6H_6	$(1.1 \pm 0.1) \times 10^8$	rt	Ad-8	S = MB, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.114.1		C_6H_5Br	3.9×10^7	0	Ad-33	$^1O_2$* from microwave discharge, A = Rub. Measured $k_Q/[(k_d/[A]) + k_A] = 0.3$ at [A] = 1.5×10^{-4} mol dm^{-3}. k_Q derived using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.3 \times 10^4$ s^{-1} [*1.34*].	Guil.73F333
10.114.2		$C_6H_5CH_3$	2.7×10^8 (est)	rt	Ad-25	S = A = Rub. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc) and $k_A = 1.7 \times 10^8$ dm^3 mol^{-1} s^{-1}.	Zwei.75P063
10.114.3		*i*-octane	1.3×10^8 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.0 \times 10^4$ s^{-1} [*1(a).6*].	Carl...72F319
10.114.4		*i*-octane	9.6×10^7 (est)	25	Ad-23	S = A = Rub. k estimated using $k_A = 7.3 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.7 \times 10^4$ s^{-1} [*1(a).6.1*].	Carl..74F341
10.114.5		hexadecane	1.3×10^8 (est)	25	Ad-33	$^1O_2$* from microwave discharge, A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 9.0 \times 10^4$ s^{-1} [*1(a).7*].	Carl...72F319
10.114.6		$CCl_4/CHCl_3$ (9:1) v:v	5.7×10^7	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 3.2 \times 10^4$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes — Continued

No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.114.7		CS_2/MeOH (98:2) v:v	$(5.0 \pm 2.5) \times 10^8$	rt	Ad-5	S = MB, A = DPBF, flash photolysis.	Floo..73F334
10.114.8		*i*-octane/ MeOH/ C_5H_5N (94:3:3) v:v:v	2.0×10^8 (est)	25	Ad-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A = Rub. k estimated using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 5.0 \times 10^4$ s^{-1}.	Carl...72F319
10.115	Ni(II) bis[1,3-bis (2-pyridylimino) isoindoline]  ≡L	$CHCl_3$	$(1.6 \pm 0.3) \times 10^8$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050
10.116	(3,11-bisacetyl-4,10-dimethyl-1,5,9,13-tetraazacyclo-pentadeca-1,3,9,11-tetraene-*N*,*N*′,*N*″,*N*‴) Ni(II)  ≡L	$CHCl_3$	$(1.6 \pm 0.3) \times 10^9$	rt	Ad-33	S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.67 \times 10^4$ s^{-1} [*1.5*].	Monr.79A050

LIGANDS 10.117 -10.121 :



10.117	Ni(II) tetraphenyl-porphine	CCl_4	$(2.0 \pm 0.6) \times 10^9$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
10.118	Cu(II) tetraphenyl-porphine	CCl_4	$(5.0 \pm 1.5) \times 10^6$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
10.119	Zn(II) tetraphenyl-porphine	CCl_4	$(4.0 \pm 1.2) \times 10^7$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
10.119.1		CCl_4	$k_r = (1.0 \pm 0.7) \times 10^4$	rt	Ad-27	S = ? k_r derived using $k_A = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*10.119*].	Kras79A010
10.120	Co(III) tetraphenyl-porphine	CCl_4	$(2.0 \pm 0.6) \times 10^9$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
10.121	acetate-Fe(III)-tetraphenyl-porphine	CCl_4	$(1.5 \pm 0.5) \times 10^9$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1}[*1.8.3*].	Kras79A010

TABLE 10. Rate constants for the quenching of singlet oxygen by transition metal complexes —Continued

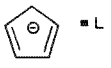
No.	Substrate (Q)	Solvent	k_q /dm^3 mol^{-1} s^{-1}	t /°C	Method	Comments	Ref.
10.122	Zn(II) tetraphenyl-chlorin	CCl_4	$(4.0 \pm 1.2) \times 10^9$	rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
10.122.1		CCl_4	$k_r = (2.0 \pm 1.4) \times 10^8$	rt	Ad-27	S = ? k derived using $k_A = 4.0 \times 10^9$ dm^3 mol^{-1} s^{-1} [*10.122*].	Kras79A010
10.123	Fe(II) bis(cyclopenta-dienyl) 	C_6H_6	$(9.0 \pm 2.0) \times 10^6$	25	Ad-8	S = An, A = DPBF, ruby laser (694 nm).	Farm.73F438
10.123.1		C_6H_6	$< 5 \times 10^6$	rt	Ad-8	S = An, A = DPBF, ruby laser (347 nm).	Wilk76F902
10.123.2		$CCl_4/CHCl_3$ (9:1) v:v	3.0×10^6	rt	Ad-23	S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 1.7 \times 10^3$ dm^3 mol^{-1} at [A] = 5×10^{-6} mol dm^{-3}. k_Q derived using $k_A = 7 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 1.43 \times 10^3$ s^{-1} [*1.8*].	Hrdl...74F645

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds

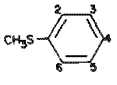
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
			[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]					
11.1	1-butanthiol $CH_3(CH_2)_2CH_2SH$	MeOH	5.9×10^4	1.7	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Mart72F519
11.2	benzylmercaptan $C_6H_5CH_2SH$	MeOH	1.4×10^5	7.3×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Mart72F519
11.3	butylmethyl sulfide $CH_3(CH_2)_2CH_2SCH_3$	$CHCl_3$	$(2.9 \pm 0.3) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.4	methylphenyl sulfide $C_6H_5SCH_3$	MeOH	$(2.0 \pm 0.1) \times 10^6$		rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.4.1		$CHCl_3$	$(2.3 \pm 0.3) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.5	benzylmethyl sulfide $C_6H_5CH_2SCH_3$	$CHCl_3$	$(1.2 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
			COMPOUNDS 11.6 - 11.13 : 					
11.6	methyl-4-fluoro-phenyl sulfide [R_4 = -F]	$CHCl_3$	$(1.9 \pm 0.2) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.7	methyl-3-chloro-phenyl sulfide [R_3 = -Cl]	$CHCl_3$	$(5.5 \pm 0.6) \times 10^5$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.8	methyl-4-chloro-phenyl sulfide [R_4 = -Cl]	MeOH	$(8.25 \pm 0.5) \times 10^5$		rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.8.1		$CHCl_3$	$(1.0 \pm 0.1) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.9	methyl-4-bromo-phenyl sulfide [R_4 = -Br]	$CHCl_3$	$(1.1 \pm 0.2) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.10	methyl-3-methyl-phenyl sulfide [R_3 = -CH_3]	$CHCl_3$	(3.1 ± 0.4) × 10^6		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7 × 10^4 s^{-1} [*1.5*].	Monr79A085
11.11	methyl-4-methyl-phenyl sulfide [R_4 = -CH_3]	MeOH	(3.1 ± 0.2) × 10^6		rt	A'd-16	S = RB, A' = DPF. k derived using k_d = 1.1 × 10^5 s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.11.1		$CHCl_3$	(4.6 ± 0.5) × 10^6		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7 × 10^4 s^{-1} [*1.5*].	Monr79A085
11.12	methyl-4-methoxy-phenyl sulfide [R_4 = -OCH_3]	MeOH	(5.3 ± 0.2) × 10^6		rt	A'd-16	S = RB, A' = DPF. k derived using k_d = 1.1 × 10^5 s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.12.1		$CHCl_3$	(7.6 ± 0.8) × 10^6		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7 × 10^4 s^{-1} [*1.5*].	Monr79A085
11.13	methyl-4-*t*-butyl phenyl sulfide [R_4 = -$C(CH_3)_3$]	$CHCl_3$	(4.7 ± 0.5) × 10^6		rt	A'd-33	S = A' = Rub. k derived using $k_{A'}$ = 5.3 × 10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7 × 10^4 s^{-1} [*1.5*].	Monr79A085
11.14	diethyl sulfide $(C_2H_5)_2S$	MeOH	4.8 × 10^6	(2.1 ± 0.6) × 10^{-2}	rt	Pa-15	S = ZnTPP. k derived using k_d = *1.0 × 10^5 s^{-1} [*1.3.6*].	Foot.71F580
11.14.1		MeOH	(1.71 ± 0.06) × 10^7		rt	A'd-16	S = RB, A' = DPF. k derived using k_d = 1.1 × 10^5 s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.14.2		C_6H_6	1.3 × 10^6	(3.2 ± 0.5) × 10^{-2}	rt	Pa-15	S = ZnTPP. k derived using k_d = *4.0 × 10^4 s^{-1} [*1.32.9*].	Foot.71F580
11.14.3		C_6H_6	4.0 × 10^6		rt	Ad-20	S = ZnTPP, A' = 9,10-di-phenylanthracene. Measured ($k/k_{A'}$) = 6.0. k derived using $k_{A'}$ = 6.7 × 10^5 dm^3 mol^{-1} s^{-1} [*3.56.8*].	Foot.71F580
11.14.4		C_6H_6	7.6 × 10^6		rt	Pa-20	S = ZnTPP, A' = Car. Measured $k_{A'}/(k_d + k[A])$ = (1.74 ± 0.05) × 10^4 dm^3 mol^{-1} at [A] = 0.1 mol dm^{-3}. k derived using $k_{A'}$ = *1.3 × 10^{10} dm^3 mol^{-1} s^{-1} [*2.130.12*] and k_d = *4.0 × 10^4 s^{-1} [*1.32.9*].	Foot.71F580
11.14.5		C_6H_6	(2.0 ± 0.2) × 10^7		rt	A'd-16	S = ZnTPP, A' = DPF. k derived using k_d = *4.0 × 10^4 s^{-1} [*1.32.9*]. Error is a 95% confidence limit.	Kach.79A086

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.14.6		C_6H_6 /MeOH (4:1)v:v	6.0×10^6 *2.3×10^6 $k_r = 3 \times 10^5$		25	P'a-20	S = MB, A' = 2M2P, P = diethylsulfoxide. k derived using $\beta_{A'} = 4.0 \times 10^{-2}$ mol dm^{-3} and k_d = 1.0×10^5 (*3.8×10^4) s^{-1} (calc).	Foot....70F734
11.15	t-butylethyl sulfide $CH_3CH_2SC(CH_3)_3$	$CHCl_3$	$(6.4 \pm 0.7) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.16	2,2'-dihydroxy-diethyl sulfide $[CH_2(OH)CH_2]_2S$	MeOH	4.0×10^6	2.5×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 5.4 kJ mol^{-1}.	Koch68F288
11.16.1		MeOH	7.7×10^6	1.3×10^{-2}	20	Od-15	S = tetrachloroeosin. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 3.8 kJ mol^{-1}.	Koch68F288
11.16.2		MeOH	6.3×10^6	1.6×10^{-2}	20	Od-15	S = tetrachloro-fluorescein. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 6.3 kJ mol^{-1}.	Koch68F288
11.16.3		MeOH	4.5×10^6	2.2×10^{-2}	20	Od-15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 7.5 kJ mol^{-1}.	Koch68F288
11.16.4		MeOH	1.0×10^7	1.0×10^{-2}	20	Od-15	S = binaphthalene-thiophene. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 8.4 kJ mol^{-1}.	Koch68F288
11.17	diisopropyl sulfide $[(CH_3)_2CH]_2S$	MeOH	$(2.51 \pm 0.03) \times 10^6$		rt	A'd-16	S = RB, A' = DPF. k derived using k_d = 1.1×10^5 s^{-1} [*1.3.4*]. Error is a 95% confidence limit.	Kach.79A086
11.17.1		$CHCl_3$	$(2.2 \pm 0.3) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.18	2-butylpropyl sulfide $CH_3CH_2CH(CH_3)SCH_2CH_2CH_3$	$CHCl_3$	$(1.1 \pm 0.2) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.19	t-butylpropyl sulfide $(CH_3)_3CSCH_2CH_2CH_3$	$CHCl_3$	$(7.2 \pm 0.8) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.20	dibutyl sulfide $[CH_3(CH_2)_2CH_2]_2S$	MeOH	9.1×10^6	1.1×10^{-2}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Mart72F519

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.20.1		$CHCl_3$	$(2.3 \pm 0.3) \times 10^7$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.20.2		EtOH	$k_r = 5.4 \times 10^6$		25	?	S = chrysene, 2-bromo-chrysene, MB. Measured $(k_q/k_r) \approx 0.7$. k_r derived using k_A(MeOH) = 9.1×10^6 dm^3 mol^{-1} s^{-1} [*11.20*].	Casa..74F648
11.21	di-2-butyl sulfide $[CH_3CH_2C(CH_3)]_2S$	$CHCl_3$	$(1.8 \pm 0.2) \times 10^6$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.22	di-*t*-butyl sulfide $[(CH_3)_3C]_2S$	MeOH	$\sim 1.5 \times 10^5$		rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*]. Theoretical intercept of 1.0 used in calculation.	Kach.79A086
11.22.1		$CHCl_3$	$(1.3 \pm 0.3) \times 10^5$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.23	diphenyl sulfide $(C_6H_5)_2S$	MeOH	$\sim 1.0 \times 10^5$		rt	A'd-16	S = RB, A' = DPF. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [*1.3.4*]. Theoretical intercept of 1.0 used in calculation.	Kach.79A086
11.23.1		$CHCl_3$	$(8.0 \pm 0.8) \times 10^4$		rt	A'd-33	S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = 1.7 \times 10^4$ s^{-1} [*1.5*].	Monr79A085
11.24	dibenzyl sulfide $(C_6H_5CH_2)_2S$	MeOH	8.3×10^6	1.2×10^{-2}	20	Od-15	S = RB, k derived using $k_d =$ *1.0×10^5 s^{-1} [*1.3.6*]. $E_a = 3.8$ kJ mol^{-1}.	Koch68F288
11.24.1		MeOH	1.5×10^7	6.7×10^{-3}	20	Od-15	S = tetrachloroeosin. k derived using $k_d =$ *1.0×10^5 s^{-1} [*1.3.6*]. $E_a = 5.4$ kJ mol^{-1}.	Koch68F288
11.24.2		MeOH	1.8×10^7	5.5×10^{-3}	20	Od-15	S = tetrachloro-fluorescein. k derived using $k_d =$ *1.0×10^5 s^{-1} [*1.3.6*]. $E_a = 1.7$ kJ mol^{-1}.	Koch68F288
11.24.3		MeOH	1.1×10^7	9.0×10^{-3}	20	Od-15	S = MB. k derived using $k_d =$ *1.0×10^5 s^{-1} [*1.3.6*]. $E_a = 7.1$ kJ mol^{-1}.	Koch68F288
11.24.4		MeOH	1.3×10^7	8.0×10^{-3}	20	Od-15	S = binaphthalene-thiophene. k derived using $k_d =$ *1.0×10^5 s^{-1} [*1.3.6*]. $E_a = 6.7$ kJ mol^{-1}.	Koch68F288

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.25	tetrahydro-thiophene 	MeOH	3.1×10^6	3.2×10^{-2}	rt	A'd–16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Mart72F519
11.25.1		$CHCl_3$	$(4.2 \pm 0.5) \times 10^7$		rt	A'd–33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7×10^4 s^{-1} [*1.5*].	Monr79A085
11.26	1-thiacyclohexane 	$CHCl_3$	$(1.3 \pm 0.2) \times 10^7$		rt	A'd–33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7×10^4 s^{-1} [*1.5*].	Monr79A085
11.27	1-oxa-4-thia-cyclohexane 	$CHCl_3$	$(1.5 \pm 0.2) \times 10^7$		rt	A'd–33	S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7×10^4 s^{-1} [*1.5*].	Monr79A085
11.28	1-thiacyclo-heptane 	$CHCl_3$	$(1.3 \pm 0.2) \times 10^7$		rt	A'd–33	S = A' Rub. k derived using $k_{A'}$ = 5.3×10^7 dm^3 mol^{-1} s^{-1} [*3.63.3*] and k_d = 1.7×10^4 s^{-1} [*1.5*].	Monr79A085
11.29	thiourea $(NH_2)_2CS$	H_2O (pH 7.1)	4.4×10^6		25	Od–19	S = phenosafranine, Q = NaN_3. k derived using k_Q = 2.0×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
11.29.1		MeOH	2.5×10^6	4.0×10^{-2}	20	Od–15	S = MB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 6.3 kJ mol^{-1}.	Koch68F288
11.30	*N*-methylthiourea $CH_3NH(NH_2)CS$	H_2O (pH 7.1)	2.0×10^6		25	Od–19	S = phenosafranine, Q = NaN_3. k derived using k_Q = 2.0×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78A360
11.31	*N*-allylthiourea $CH_2{=}CHCH_2NH(NH_2)CS$	H_2O	4.4×10^8	9.9×10^{-4}	rt	Od–14	S = proflavin. k derived using k_d = *4.4×10^5 s^{-1} [*1.1.3*].	Sluy61F008
11.31.1		H_2O (pH 7.1)	4.0×10^6		25	Od–19	S = phenosafranine, Q = NaN_3. k derived using k_Q = 2×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*].	Kral.78F020
11.31.2		H_2O (pH 7.0)	4.5×10^6		rt	Od–19	S = chlorophyll-a, Q = N_3^-. k derived using k_Q = 2×10^8 dm^3 mol^{-1} s^{-1} [*12.9.6*]. S solubilized in Triton X-100 micelles (1.0 % by volume).	Barb.78A278
11.31.3		MeOH	1.0×10^6	1.0×10^{-1}	20	Od–15	S = chlorophyll-a. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Livi.56F005

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

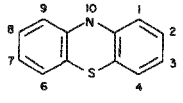
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.31.4		C_5H_5N	$\approx 2.7 \times 10^7$		12	P'a-20	S = A' = DMA. Measured ($k/k_{A'}$) = 0.7. k derived using (k(TME)/$k_{A'}$) = 1.1 and k(TME) = 4.0×10^7 dm^3 mol^{-1} s^{-1} [*2.35.3*].	Kram.73F202
				COMPOUNDS 11.32 - 11.34 :				
								
11.32	4*H*-pyran-4-thione	CH_2Cl_2	7.5×10^6	$(1.6 \pm 0.5) \times 10^{-3}$	25	Pa-15	S = MB, P = 4*H*-pyran-4-ketone. k derived using k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Ishi..71F403
11.33	2,6-dimethyl-4*H*-pyran-4-thione [$R_2 = R_6 = -Me$]	CH_2Cl_2	4.0×10^7	$(3.0 \pm 0.9) \times 10^{-4}$	25	Pa-15	S = MB, P = 2,6-dimethyl-4*H*-pyran-4-ketone. k derived using k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Ishi..71F403
11.34	2,6-diphenyl-4*H*-pyran-4-thione [$R_2 = R_6 = -Ph$]	CH_2Cl_2	8.6×10^6	$(1.4 \pm 0.2) \times 10^{-3}$	25	Ad-15	S = MB, k derived using k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Ishi..71F403
11.35	thiophene 	MeOH	$\leqslant 1.7 \times 10^2$	$\geqslant 6.0 \times 10^2$	20	Od-15	S = RB, k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 25 kJ mol^{-1}.	Koch68F288
11.35.1		MeOH	2.2×10^5	4.5×10^{-1}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Mart72F519
				COMPOUNDS 11.36 - 11.38 :				
								
11.36	phenothiazine [$R_{10} = -H$]	MeOH /C_6H_6 (9:1) v:v	4.5×10^7	β_r = 2.2×10^{-3} (est)	15	Pa-17 P'a (sep)	S = MB, Measured (β_r/β_r(MeOH)) = 0.94. β_r estimated using k_r = 4.2×10^7 dm^3 mol^{-1} s^{-1} [*11.36.5*] and k_d(MeOH) = *1.0×10^5 s^{-1} [*1.3.6*]. k_r derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Ram...75F623
11.36.1		MeOH /C_6H_6 (4:1) v:v	2.6×10^7 (est)	β_r = 2.4×10^{-3} (est)	15	Pa-17 P'a (sep)	S = MB. Measured (β_r/β_r(MeOH)) = 1.0. β_r estimated using k_r = 4.2×10^7 dm^3 mol^{-1} s^{-1} [*11.36.5*] and k_d(MeOH) = *1.0×10^5 s^{-1} [*1.3.6*]. k_r estimated using k_d = 9.4×10^4 s^{-1} (calc).	Ram...75F623

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.36.2		MeOH /C_6H_6 (1:4) v:v	1.7×10^7 (est)	$\beta_r = 3.6 \times 10^{-3}$ (est)	15	Pa-17 P'a (sep)	S = MB. Measured (β_r/β_r(MeOH)) = 1.5. β_r estimated using $k_r = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*11.36.5*] and k_d(MeOH) = *1.0×10^5 s^{-1} [*1.3.6*]. k_r estimated using $k_d = 6.13 \times 10^4$ s^{-1} (calc).	Ram...75F623
11.36.3		MeOH /glycol (3:1) v:v	9.2×10^7 (est)	$\beta_r = 1.2 \times 10^{-3}$	15	Pa-17 P'a (sep)	S = MB. Measured (β_r/β_r(MeOH)) = 0.51. β_r estimated using $k_r = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*11.36.5*] and k_d(MeOH) = *1.0×10^5 s^{-1} [*1.3.6*]. k_r estimated using $k_d = 1.1 \times 10^5$ s^{-1} (calc).	Ram...75F623
11.36.4		MeOH /glycol (1:3) v:v	1.8×10^8 (est)	$\beta_r = 8.0 \times 10^{-4}$	15	Pa-17 P'a (sep)	S = MB. Measured (β_r/β_r(MeOH)) = 0.34. β_r estimated using $k_r = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*11.36.5*] and k_d(MeOH) = *1.0×10^5 s^{-1} [*1.3.6*]. k_r estimated using $k_d = 1.4 \times 10^5$ s^{-1} (calc).	Ram...75F623
11.36.5		C_6H_5Br /MeOH (2:1) v:v	4.2×10^7 (est)		rt	A'd-23	S = A' = Rub. k estimated using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.89 \times 10^4$ s^{-1} (calc).	Rose..77F240
11.37	10-methylphenothiazine [R_{10} = -Me]	C_6H_5Br /MeOH (2:1) v:v	$\leqslant 1.2 \times 10^6$ (est)		rt	A'd-23	S = A' = Rub. k estimated using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.89 \times 10^4$ s^{-1} (calc).	Rose..77F240
11.38	chloropromazine [R_3 = -Cl, R_{10} = $-(CH_2)_3N(CH_3)_2$]	C_6H_5Br /MeOH (2:1) v:v	3.5×10^7 (est)		rt	A'd-23	S = A' = Rub. k estimated using $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 4.89 \times 10^4$ s^{-1} (calc).	Rose..77F240
11.39	diethyl disulfide $C_2H_5SSC_2H_5$	MeOH	1.8×10^7	5.5×10^{-3}	rt	A'd-16	S = MB, A' = DPBF. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Mart72F519
11.40	1,4-dithiane 	CH_3CN	5.1×10^5	$\sim 5.0 \times 10^{-2}$	rt	Pa-15	S = RB. k derived using k_d = *2.55×10^4 s^{-1} [*1.17*]. Slope estimated as tangent to curve.	Foot.71F580
11.40.1		CH_3CN	2.6×10^6	$(9.8 \pm 0.7) \times 10^{-3}$	rt	Pa-15	S = RB. k derived using k_d = *2.55×10^4 s^{-1} [*1.17.2*]. Solvent contained 0.05% H_2O by molarity.	Foot.71F580
11.40.2		CH_3CN	1.5×10^6	$(1.7 \pm 0.2) \times 10^{-2}$	rt	Pa-15	S = RB. k derived using k_d = *2.55×10^4 s^{-1} [*1.17.2*]. Solvent contained 0.52% H_2O by molarity.	Foot.71F580

TABLE 11. Rate constants for the interaction of singlet oxygen with sulfur containing compounds — Continued

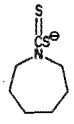
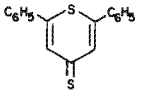
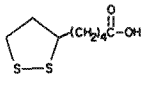
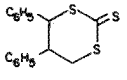
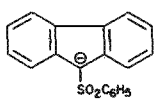
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
11.40.3		CH_3CN/H_2O (95:5) Mole %	6.3×10^6 (est)	$(6.7 \pm 0.1) \times 10^{-3}$	rt	Pa-15	S = RB. k estimated using $k_d = 4.2 \times 10^4$ s^{-1} (calc).	Foot.71F580
11.40.4		CH_3CN/H_2O (61:39) Mole %	1.1×10^7 (est)	$(1.7 \pm 0.2) \times 10^{-2}$	rt	Pa-15	S = RB. k estimated using $k_d = 1.9 \times 10^5$ s^{-1} (calc).	Foot.71F580
11.41	dimethyldithiocarbamate ion $(CH_3)_2NCSS^-$	H_2O (pH 7.1)	$\approx 8.0 \times 10^7$		25	Od-19	S = phenosaframine, Q = NaN_3. k derived using $k_Q = 2.0 \times 10^8$ dm^3 mol^{-1}s^{-1} [*12.9.6*].	Kral.78A360
11.42	hexamethylenedithiocarbamate 	EtOH	1.5×10^8		rt	Od-23	S = RB, A′ = Car. Measured $k_{A'}/(k_d + k_A[A]) = 7 \times 10^4$ dm^3 mol^{-1} at [A] = 3.35×10^{-4} mol dm^{-3}. k derived using $k_{A'} = 5.0 \times 10^9$ dm^3 mol^{-1} s^{-1} and $k_d = 1.0 \times 10^4$ s^{-1}.	Yama..72F116
11.43	4*H*-thiopyran-4-thione 	CH_2Cl_2	$> 1.2 \times 10^8$	$< 1.0 \times 10^{-4}$	25	Pa-15	S = MB, P = 4*H*-thiopyran-4-ketone. k derived using $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Ishi..71F403
11.44	2,6-diphenyl-4*H*-thiopyran-4-thione 	CH_2Cl_2	4.6×10^6	$(2.6 \pm 0.3) \times 10^{-3}$	25	Ad-15	S = MB. k derived using $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Ishi..71F403
11.45	lipoic acid 	C_6H_6	1.0×10^8	$(3.5 \pm 0.5) \times 10^{-4}$	25	A′d-23	S = A′ = Rub. k derived using $k_d = 4.2 \times 10^4$ s^{-1} [*1.32*].	Stev..74F641
				For more relative rates see		3.63.20.		
11.46	4,5-diphenyl 1,3-dithiole-2-thione 	C_6H_6 /MeOH (5:1) v:v	3.6×10^7 (est)	1.4×10^{-3}	20	Od-15	S = MB, k estimated using $k_d = 5.0 \times 10^4$ s^{-1} (calc).	Fang.77F794
11.47	9-benzenesulfonyl-fluoren-9-yl anion 	*t*-BuOH	6.5×10^7	$(4.6 \pm 0.2) \times 10^{-4}$	30	Pa-15	S = RB, P = fluorenone. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Bete.70F250
11.47.1		*t*-BuOH	7.9×10^7	$(3.8 \pm 0.3) \times 10^{-4}$	30	Pa-15	S = self, P = fluorenone. k derived using $k_d = 3.0 \times 10^4$ s^{-1} [*1.25*].	Bete.70F250

TABLE 12. Rate constants for the interaction of singlet oxygen with some inorganic compounds

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
	[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]							
12.1	chloride ion $[CH_3(CH_2)_2CH_2]_4NCl$	C_6H_5Br /Me_2CO (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.1.1		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.2	bromide ion LiBr	C_6H_5Br /Me_2CO (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.2.1		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.3	bromide ion $[CH_3(CH_2)_2CH_2]_4NBr$	C_6H_5Br /Me_2CO (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.3.1		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.4	bromide ion (dicyclohexano-18-crown-6-polyether potassium bromide)	C_6H_5Br /Me_2CO (est) (2:1) v:v	$\approx 1.2 \times 10^6$		rt	A′d–23	S = A′ = Rub. k estimated using $k_d = 3.24 \times 10^4$ s^{-1} (calc) and $k_{A^\cdot} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Rose.76F126
12.5	iodide ion LiI	C_6H_5Br /Me_2CO (est) (2:1) v:v	$(8.1 \pm 0.1) \times 10^7$		rt	A′d–23	S = A′ = Rub. k estimated using $k_d = 3.24 \times 10^4$ s^{-1} (calc) and $k_{A^\cdot} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1}.	Rose.76F126
12.5.1		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d–23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.6	iodide ion KI	H_2O	7.2×10^6		28	Pa–23	S = 1-anthracene-sulfonate ion, Q = NaN_3, P = I_3^-. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*] and $k_Q = 2.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Roha.77F074
12.6.1		H_2O	6.4×10^6		28	Pa–23	S = 2-anthracene-sulfonate ion, Q = NaN_3, P = I_3^-. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*] and $k_Q = 2.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Roha.77F074
12.6.2		H_2O	7.2×10^6		28	Pa–23	S = 1,5-anthracene-disulfonate ion, Q = NaN_3, P = I_3^-. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*] and $k_Q = 2.2 \times 10^8$ dm^3 mol^{-1} s^{-1} [*12.9.6*].	Roha.77F074
12.6.3		H_2O	8.65×10^6	5.8×10^{-2}	rt	Pa–23	S = A′ = 1-anthracene sulfonate, Q = N_3^-, P = I_3^-. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Gupt.78F183

TABLE 12. Rate constants for the interaction of singlet oxygen with some inorganic compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
12.6.4		H_2O/MeOH (4:1) v:v	5.55×10^6 (est)	7.2×10^{-2}	rt	Pa-23	S = A′ = 1-anthracene sulfonate, Q = N_3^-, P = I_3^-. k estimated using $k_d = 4.0\times10^5$ s^{-1} (calc).	Gupt.78F183
12.6.5		H_2O/MeOH (3:2) v:v	2.98×10^6 (est)	1.1×10^{-1}	rt	Pa-23	S = A′ = 1-anthracene sulfonate, Q = N_3^-, P = I_3^-. k estimated using $k_d = 3.2\times10^5$ s^{-1} (calc).	Gupt.78F183
12.6.6		H_2O/MeOH (2:3) v:v	1.54×10^6 (est)	1.6×10^{-1}	rt	Pa-23	S = A′ = 1-anthracene sulfonate, Q = N_3^-, P = I_3^-. k estimated using $k_d = 2.5\times10^5$ s^{-1} (calc).	Gupt.78F183
12.6.7		H_2O/MeOH (1:4) v:v	3.4×10^5 (est)	5.6×10^{-1}	rt	Pa-23	S = A′ = 1-anthracene sulfonate, Q = N_3^-, P = I_3^-. k estimated using $k_d = 1.9\times10^5$ s^{-1} (calc).	Gupt.78F183
12.6.8		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d-23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.7	iodide ion $[CH_3(CH_2)_2CH_2]_4NI$	C_6H_5Br /Me_2CO (2:1) v:v	$(9.1\pm0.1)\times10^7$ (est)		rt	A′d-23	S = A′ = Rub. k estimated using $k_d = 3.24\times10^4$ s^{-1} (calc) and $k_{A'}$ = 4×10^7 dm^3 mol^{-1} s^{-1}.	Rose.76F126
12.7.1		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A′d-23	S = A′ = Rub. No measurable effect.[a]	Rose.76F126
12.8	iodide ion (dicyclohexano-18-crown-6-polyether potassium iodide)	C_6H_5Br /Me_2CO (2:1) v:v	$(2.8\pm0.1)\times10^8$ (est)		rt	A′d-23	S = A′ = Rub. k estimated using $k_d = 3.24\times10^4$ s^{-1} (calc) and $k_{A'}$ = 4×10^7 dm^3 mol^{-1} s^{-1}.	Rose.76F126
12.9	azide ion NaN_3	H_2O	7.9×10^8		40	A′d-23	S = Py, A′ = DPBF. k derived using k_d = 5.0×10^5 s^{-1} [*I.I*]. A′ and S solubilized in SDS micelles.	Miyo.78A174
12.9.1		H_2O	1.8×10^9		40	A′d-23	S = Py, A′ = DPBF. k derived using k_d = 5.0×10^5 s^{-1} [*I.I*]. A′ and S solubilized in SDS micelles.	Miyo.78A174
12.9.2		H_2O (pH 8.4)	$(1.7\pm0.2)\times10^9$		25	A′d-20	S = MB, A′ = trypto-phan. k derived using $\beta_{A'}$ = ? and k_d = 5.0×10^5 s^{-1} [*I.I*].	Usui..78F061
12.9.3		H_2O (pH 7.0)	$(2.2\pm0.3)\times10^9$		25	A′d-20	S = MB, A′ = diphenyl-oxazole. k derived using $\beta_{A'}$ = ? and k_d = 5.0×10^5 s^{-1} [*I.I*]. A′ solubilized in DTAC micelles.	Usui..78F061

TABLE 12. Rate constants for the interaction of singlet oxygen with some inorganic compounds — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
12.9.4		H_2O (pH 7.0)	$(2.3 \pm 0.3) \times 10^9$		25	A'd-20	S = MB, A' = DMA. k derived using $\beta_{A'} = ?$ and $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. A' solubilized in DTAC micelles.	Usui..78F061
12.9.5		H_2O	2.08×10^9		rt	P"a-23	S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3^-. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*].	Gupt.78F183
12.9.6		MeOH	2.2×10^8		rt	A'd-5	S = MB, A' = DPBF, ruby laser (610 nm).	Hast...72F515
12.9.7		MeOH	2.3×10^8 *1.6×10^8		rt	A'd-23	S = Py, A' = DPBF. k derived using $k_d = 1.4 \times 10^5$ (*1.0×10^5) s^{-1} [*1.3*].	Miyo.78A174
12.9.8		H_2O/MeOH (4:1) v:v	1.33×10^9 (est)		rt	P"a-23	S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3^-. k estimated using $k_d = 4.0 \times 10^5$ s^{-1} (calc).	Gupt.78F183
12.9.9		H_2O/MeOH (3:2) v:v	1.13×10^9 (est)		rt	P"a-23	S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3^-. k estimated using $k_d = 3.2 \times 10^5$ s^{-1} (calc).	Gupt.78F183
12.9.10		H_2O/MeOH (2:3) v:v	5.2×10^8 (est)		rt	P"a-23	S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3^-. k estimated using $k_d = 2.5 \times 10^5$ s^{-1} (calc).	Gupt.78F183
12.9.11		H_2O/MeOH (1:4) v:v	3.0×10^8 (est)		rt	P"a-23	S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3^-. k estimated using $k_d = 1.9 \times 10^5$ s^{-1} (calc).	Gupt.78F183
12.10	superoxide ion $[(CH_3)_4N]O_2$	CH_3CN	$(7 \pm 6) \times 10^9$ *6.6×10^9	$(5.0 \pm 4.3) \times 10^{-6}$	rt	A'd-16	S = RB, A' = DPBF. k derived using $k_d = 3.3 \times 10^4$ (*2.55×10^4) s^{-1} [*1.17*].	Guir.76E072
12.10.1		Me_2SO	1.6×10^9 (est)	$(3.3 \pm 0.5) \times 10^{-5}$	rt	A'd-16	S = RB, A' = DPBF. k estimated using $k_d = 5.2 \times 10^4$ s^{-1} [*1(a).1*].	Guir.76E072
12.11	superoxide ion $([CH_3(CH_2)_2CH_2]_4N)O_2$	C_6H_5Br /CH_3CN (2:1) v:v	$(3.6 \pm 0.1) \times 10^7$ (est)		rt	A'd-23	S = A' = Rub. k estimated using $k_d = 3.07 \times 10^4$ s^{-1} (calc) and $k_{A'} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1}. Showed $k_q >> k_r$.	Rose75F578

[a]The salt may not be completely dissociated in this solvent.

TABLE 13. Rate constants for the interaction of singlet oxygen with nitrones, azodioxides, and nitroso compounds

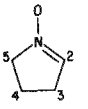
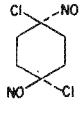
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
	[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]							
13.1	acetone oxime $(CH_3)_2C{=}NOH$	MeOH	$k_r \leqslant 1.0 \times 10^4$ *1.2×10^4		rt	A'd-17 Pa	S = RB, A' = 2M2B, P = acetophenone. Measured ($k_r/k_r^{A'}$) = 7.7×10^{-3}. k_r derived using $k_r^{A'}$ = 1.3×10^6 (*1.5×10^6) dm^3 mol^{-1} s^{-1} [*A3.1*].	Wams.76F197
13.2	benzophenone oximate anion $(C_6H_5)_2C{=}NO^-$	MeOH	$k_r = 3.4 \times 10^5$ *3.9×10^5		rt	A'd-17 Pa	S = RB, A' = 2M2B, P = benzophenone. Measured ($k_r/k_r^{A'}$) = 0.26. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ (*1.5×10^6) dm^3 mol^{-1} s^{-1} [*A3.1*].	Wams.76F197
13.3	benzophenone oxime $(C_6H_5)_2C{=}NOH$	MeOH	$k_r = 7.7 \times 10^4$ *8.9×10^4		rt	A'd-17 Pa	S = RB, A' = 2M2B, P = benzophenone. Measured ($k_r/k_r^{A'}$) = 5.9×10^{-2}. k_r derived using $k_r^{A'}$ = 1.3×10^6 (*1.5×10^6) dm^3 mol^{-1} s^{-1} [*A3.1*].	Wams.76F197
13.4	benzophenone oxime-*O*-methyl ether $(C_6H_5)_2C{=}NOCH_3$	MeOH	$k_r = 2.0 \times 10^5$ *2.3×10^5		rt	A'd-17 Pa	S = RB, A' = 2M2B, P = benzophenone. Measured ($k_r/k_r^{A'}$) = 0.15. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ (*1.5×10^6) dm^3 mol^{-1} s^{-1} [*A3.1*].	Wams.76F197
	COMPOUNDS 13.5 and 13.6: 							
13.5	4,5,5-trimethyl-Δ^1-pyrroline-*N*-oxide [$R_4 = R_5 = R_5 = -Me$]	$CHCl_3$	5×10^7		rt	A'd-16	S = MB, A' = DPBF. k derived using k_d (unreported). $k = k_q$ (No reaction observed).	Chin.75F653
13.6	2,4,4-trimethyl-Δ^1-pyrroline-*N*-oxide [$R_2 = R_4 = R_4 = -Me$]	$CHCl_3$	2.1×10^7		rt	A'd-16	S = MB, A' = DPBF. k derived using k_d(unreported).	Chin..75F653
13.7	2-methyl-2-nitroso-propane $(CH_3)_3CNO$	CH_2Cl_2 /MeOH (15:1) v:v	9.3×10^9 (est)		rt	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'}$ = 4.0×10^7 dm^3 mol^{-1} s^{-1} and $k_d = 1.1 \times 10^4$ s^{-1} [*1(a).10*].	Sing.76F900
13.8	*trans*-1,4-dichloro-1,4-dinitrosocyclo-hexane 	CH_2Cl_2 /MeOH (11:5) v:v	5.3×10^9 (est)		rt	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'}$ = 4.0×10^7 dm^3 mol^{-1} s^{-1} and $k_d = 1.9 \times 10^4$ s^{-1} [*1(a).9*].	Sing.76F900

TABLE 13. Rate constants for the interaction of singlet oxygen with nitrones, azodioxides, and nitroso compounds — Continued

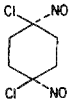
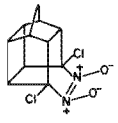
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
13.9	*cis*-1,4-dichloro-1,4-dinitrosocyclohexane 	CH_2Cl_2 /MeOH (11:5) v:v	9.2×10^9 (est)		rt	A'd-32	S = chlorophyll-a, A' = DPBF. k estimated using $k_A' = 8 \times 10^8$ dm^3 mol^{-1} s^{-1} [*5.36.9*] and $k_d = 2.1 \times 10^4$ s^{-1} [*1(a).9*]. Assumed that quenching is due to 13.9 in equilibrium with 13.10.	Sing.76F900
13.9.1		CH_2Cl_2 /MeOH (11:5) v:v	1.2×10^{10} (est)		rt	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.1 \times 10^4$ s^{-1} [*1(a).9*]. Assumed quenching is due to 13.9 in equilibrium with 13.10.	Sing.76F900
13.10	1,4-dichloro-2,3-diazabicyclo-[2.2.2]-oct-2-ene-2,3-dioxide 	CH_2Cl_3 /MeOH (11:5) v:v	8.0×10^7 (est)		rt	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.1 \times 10^4$ s^{-1} [*1(a).9*]. Assumed quenching is due to 13.10 only. (See 13.9)	Sing.76F900
13.11		CH_2Cl_2 /MeOH (11:5) v:v	$< 2 \times 10^6$ (est)		rt	A'd-32	$^1O_2$* from $(PhO)_3PO_3$ decomp., A' = Rub. k estimated using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 2.1 \times 10^4$ s^{-1} [*1(a).9*].	Sing.76F900

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest

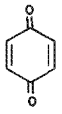
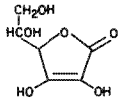
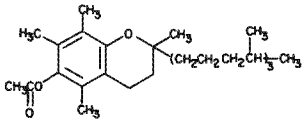
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
	[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]							
14.1	benzoquinone 	EtOH	3.4×10^7 (est)		rt	A'd-19	S = RB, A' = chlorophyll-a. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
14.1.1		C_6H_6/EtOH (2:1) v:v	1.62×10^7 (est)		rt	A'd-19	S = RB, A' = chlorophyll-a. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
14.2	ascorbic acid 	MeOH	8.3×10^6	1.2×10^{-2}	20	Od-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*]. E_a = 63 kJ mol^{-1}.	Koch68F288
14.3	α-tocopheryl acetate 	C_5H_5N	$\leqslant 1.6 \times 10^6$		rt	A'd-23	S = A' = Rub. k derived using $k_{A\cdot} = 4 \times 10^7$ dm^3 mol^{-1} s^{-1} and k_d = *6.0×10^4 s^{-1} [*1.29.1*].	Fahr...74R112
14.4	methyl stearate $CH_3(CH_2)_{16}COOCH_3$	C_5H_5N	$k_r \leqslant 5 \times 10^4$		rt	Ad-17 A'd	S = protoporphyrin, A' = cholesterol. No measurable effect.	Dole...74R115
14.5	methyl oleate $CH_3(CH_2)_7CH{=}CH(CH_2)_7COOCH_3$	EtOH	1.3×10^5	6.3×10^{-1}	20	Pa-15	S = MB, P = methyloleatemonohydroperoxide. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*].	Tera.77F378
14.5.1		C_5H_5N	$k_r = 7.3 \times 10^6$		rt	Ad-17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 1.1. k_r derived using $k_r^{A'} = k_{A\cdot} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
14.5.2		C_5H_5N	$k_r = 9.2 \times 10^4$		rt	Ad-17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 1.4. k_r derived using $k_r^{A'} = k_{A\cdot} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
14.6	methyl linoleate $CH_3(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_7COOCH_3$	EtOH	2.2×10^5	3.6×10^{-1}	20	Pa-15	S = MB, P = methyllinoleatemonohydroperoxide. k derived using k_d = *7.9×10^4 s^{-1} [*1.10.3*].	Tera.77F378
14.6.1		C_5H_5N	$k_r = 1.2 \times 10^5$		rt	Ad-17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 1.9. k_r derived using $k_r^{A'} = k_{A\cdot} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

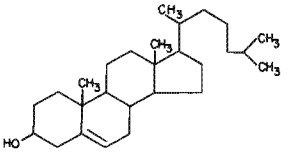
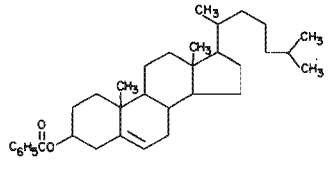
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.6.2		C_5H_5N	$k_r = 1.3 \times 10^5$		rt	Ad–17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 2.0 ± 0.2. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*A3.19*].	Dole...74F115
			For more relative rates see		4.25.2, 4.27.2, 4.28.6.			
14.7	methyl linolenate	EtOH	2.9×10^5	2.7×10^{-1}	20	Pa–15	S = MB, P = methyl-linolenatemonohydro-peroxide. k derived using k_d = *7.9 × 10^4 s^{-1} [*1.10.3*].	Tera.77F378
	$CH_3(CH_2CH{=}CH)_3CH_2(CH_2)_6COOCH_3$							
14.7.1		C_5H_5N	$k_r = 1.9 \times 10^5$		rt	Ad–17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 2.9. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
14.7.2		C_5H_5N	$k_r = 1.8 \times 10^5$		rt	Ad–17 A'd	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 2.7. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
14.7.3		C_5H_5N	1.6×10^5		rt	A'd–23	S = A' = Rub. k derived using $k_{A'} = 4.0 \times 10^7$ dm^3 mol^{-1} s^{-1} and $k_d = 6.0 \times 10^4$ s^{-1} [*1.29.1*].	Dole...74R115
14.8	methyl arachidonate	C_5H_5N	$k_r = 2.2 \times 10^5$		rt	Ad–17 A'd (sep)	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 3.4. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
	$CH_3(CH_2)_4(CH{=}CHCH_2)_4CH_2CH_2COOCH_3$							
14.8.1		C_5H_5N	$k_r = 2.9 \times 10^5$		rt	Ad–17 A'd	S = protoporphyrin, A' = cholesterol. Measured ($k_r/k_r^{A'}$) = 4.4. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm^3 mol^{-1} s^{-1} [*14.9*].	Dole...74R115
14.9	cholesterol	C_5H_5N	6.6×10^4	8.94×10^{-1}	20	Od–15	S = hematoporphyrin. k derived using k_d = *5.9 × 10^4 s^{-1} [*1.29.1*].	Sche..57F008
								
			For more relative rates see		14.4, 14.5.1–2, 14.6.1–2, 14.7.1–2, 14.8, 14.8.1.			
14.10	cholesteryl benzoate	C_6H_6 /C_5H_5N (10:1) v:v	1.1×10^4 (est)	3.98	20	Od–15	S = hematoporphyrin. k estimated using $k_d = 4.2 \times 10^4$ s^{-1} (calc).	Sche..57F008
								

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

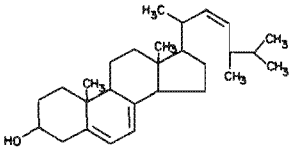
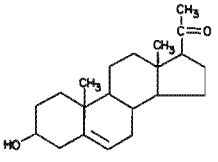
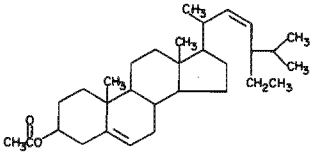
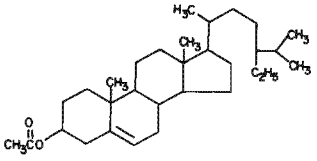
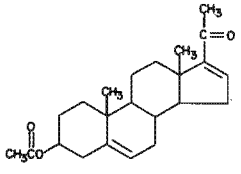
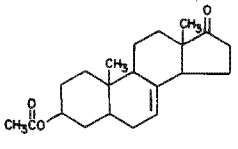
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.11	ergosterol 	C_5H_5N	1.3×10^7	4.5×10^{-3}	20	Od-15	S = hematoporphyrin. k derived using k_d = *5.9 × 10^4 s^{-1} [*1.29.1*].	Sche..57F008
14.12	pregnenolone 	C_5H_5N	3.5×10^4	1.71	20	Od-15	S = hematoporphyrin. k derived using k_d = *5.9 × 10^4 s^{-1} [*1.29.1*].	Sche.58F002
14.12.1		C_6H_6 /C_5H_5N (3:2) v:v	2.7×10^4 (est)	1.79	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.8 × 10^4 s^{-1} (calc).	Sche..58F002
14.12.2		C_6H_6 /C_5H_5N (5:2) v:v	2.5×10^4 (est)	1.82	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.6 × 10^4 s^{-1} (calc).	Sche..57F008
14.13	stigmasteryl acetate 	C_6H_6 /C_5H_5N (10:1) v:v	1.0×10^4 (est)	4.06	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.2 × 10^4 s^{-1} (calc).	Sche..57F008
14.14	sitosteryl acetate 	C_6H_6 /C_5H_5N (10:1) v:v	6.5×10^3 (est)	6.50	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.2 × 10^4 s^{-1} (calc).	Sche..57F008
14.15	16-dehydropregnenolone-3-acetate 	C_6H_6 /C_5H_5N (10:1) v:v	9.0×10^3 (est)	4.65	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.2 × 10^4 s^{-1} (calc).	Sche..57F008
14.16	7-dehydroandrosterone-3-acetate 	C_6H_6 /C_5H_5N (10:1) v:v	6.6×10^3 (est)	6.34	20	Od-15	S = hematoporphyrin. k estimated using k_d = 4.2 × 10^4 s^{-1} (calc).	Sche..57F008

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

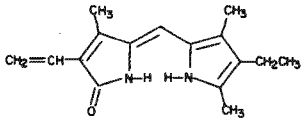
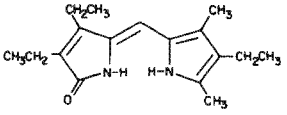
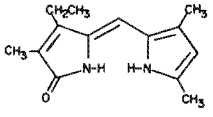
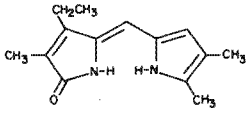
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.17	5′-oxo-4′-vinyl-4-ethyl-3′,3,5-trimethyl-1′,5′-dihydro-(2.2′)-dipyrromethene 	MeOH	2.2×10^9		rt	Ad-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.17.1		MeOH	$k_r = 8.5 \times 10^8$		rt	Ad-15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.17.2		$CHCl_3$	2.2×10^9 $*1.3 \times 10^9$		rt	Ad-15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.17.3		$CHCl_3$	$k_r = 1.9 \times 10^9$ $*1.1 \times 10^9$		rt	Ad-15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.18	5′-oxo-3′,4′,4-triethyl-3,5-dimethyl-1′,5′-dihydro-(2.2′)-dipyrromethene 	MeOH	1.9×10^9		rt	Ad-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.18.1		MeOH	$k_r = 9.9 \times 10^8$		rt	Ad-15	S = RB. k derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.18.2		$CHCl_3$	4.2×10^9 $*2.5 \times 10^9$		rt	Ad-15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.18.3		$CHCl_3$	$k_r = 3.2 \times 10^9$ $*1.9 \times 10^9$		rt	Ad-15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.19	5′-oxo-3′-ethyl-4′,3,5-trimethyl-1,5′-dihydro-(2.2′)-dipyrromethene 	MeOH	7.9×10^8		rt	Ad-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.19.1		MeOH	$k_r = 4.3 \times 10^8$		rt	Ad-15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.19.2		$CHCl_3$	2.4×10^9 $*1.4 \times 10^9$		rt	Ad-15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.19.3		$CHCl_3$	$k_r = 1.6 \times 10^9$ $*9.3 \times 10^8$		rt	Ad-15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.20	5′-oxo-4′,4,5-trimethyl-3′-ethyl-1,5′-dihydro-(2.2′)-dipyrromethene 	MeOH	1.6×10^9		rt	Ad-15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.20.1		MeOH	$k_r = 6.2 \times 10^8$		rt	Ad-15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

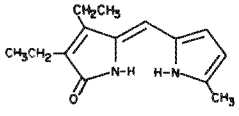
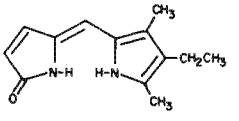
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.20.2		$CHCl_3$	2.5×10^9 $*1.5 \times 10^9$		rt	Ad–15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.20.3		$CHCl_3$	$k_r = 1.7 \times 10^9$ $*1.0 \times 10^9$		rt	Ad–15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.21	5′–oxo–3′,4′–di–ethyl–5–methyl–1, 5′–dihydro–(2.2′) dipyrromethene 	MeOH	5.7×10^8		rt	Ad–15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.21.1		MeOH	$k_r = 2.1 \times 10^8$		rt	Ad–15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.21.2		$CHCl_3$	1.5×10^9 $*9.0 \times 10^8$		rt	Ad–15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.21.3		$CHCl_3$	$k_r = 8.0 \times 10^8$ $*4.8 \times 10^8$		rt	Ad–15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.22	5′–oxo–4–ethyl–3,5–dimethyl–1, 5′–dihydro–(2.2′)–dipyrromethene 	MeOH	1.4×10^8		rt	Ad–15	S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104
14.22.1		MeOH	$k_r = 7.0 \times 10^7$		rt	Ad–15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.22.2		$CHCl_3$	4.4×10^9 $*2.6 \times 10^9$		rt	Ad–15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.22.3		$CHCl_3$	$k_r = 3.0 \times 10^9$ $*1.8 \times 10^9$		rt	Ad–15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

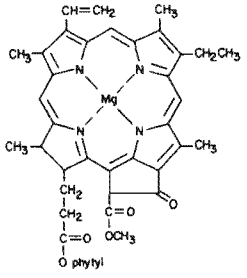
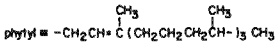
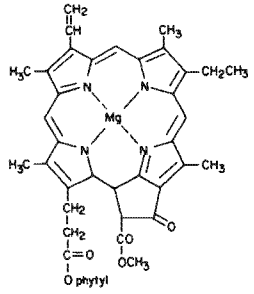
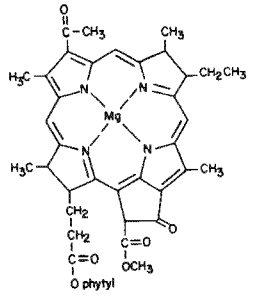
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.23	chlorophyll-a	CCl_4	$(7.0 \pm 2.1) \times 10^8$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
								
								
14.23.1		CCl_4	$k_r = (4.0 \pm 2.8) \times 10^6$		rt	Ad-27	S = ? k_r derived using $k_A = 7.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*14.23*].	Kras79A010
14.23.2		EtOH	1.98×10^7 (est)	5.02×10^{-3}	rt	Ad-15	S = RB. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
14.23.3		C_6H_6/EtOH (2:1) v:v	1.2×10^7 (est)		rt	Ad-19	S = RB, A′ = Car. k estimated using $k_d = 1 \times 10^5$ s^{-1} (calc).	Koka.78F404
14.24	protochlorophyll	CCl_4	$< 1 \times 10^8$ (est)		rt	Ld-13	S = ? k estimated using $k_d = 3.6 \times 10^1$ s^{-1}[*1.8.3*]. Analysis complicated by a protopheophytin impurity.	Kras79A010
								
14.24.1		CCl_4	$k_r < 1 \times 10^6$ (est)		rt	Ad-27	S = ? k_r estimated using $k_A = 1.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*14.24*].	Kras79A010
14.25	bacterio-chlorophyll-a	CCl_4	$(1.0 \pm 0.3) \times 10^9$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
								

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

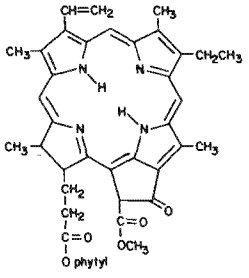
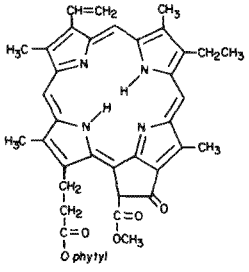
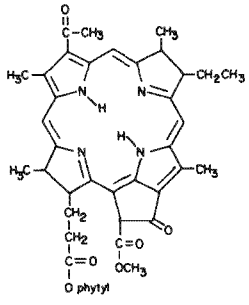
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.26	pheophytin-a	CCl_4	$(2.0 \pm 0.6) \times 10^7$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
								
14.26.1		CCl_4	$k_r = (1.0 \pm 0.7) \times 10^4$		rt	Ad-27	S = ? k_r derived using $k_A = 2.0 \times 10^7$ dm^3 mol^{-1} s^{-1} [*14.26*].	Kras79A010
14.27	protopheophytin	CCl_4	$(2.0 \pm 0.6) \times 10^8$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
								
14.27.1		CCl_4	$k_r \approx (1.0 \pm 0.7) \times 10^8$		rt	Ad-27	S = ? k_r derived using $k_A = 2.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*14.27*].	Kras79A010
14.28	bacterio-pheophytin-a	CCl_4	$(1.0 \pm 0.3) \times 10^7$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
								

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

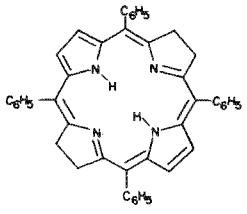
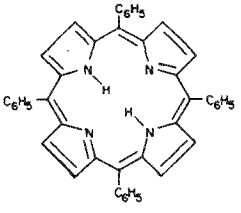
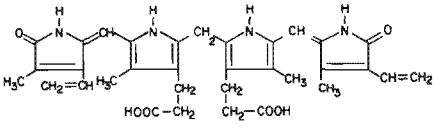
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.29	tetraphenylbacteriochlorin-*trans* 	CCl_4	$(1.0 \pm 0.3) \times 10^8$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
14.29.1		CCl_4	$k_r = 2 \times 10^5$		rt	Ad-27	S = ? k_r derived using $k_A = 1.0 \times 10^8$ dm^3 mol^{-1} s^{-1} [*14.29*].	Kras79A010
14.30	tetraphenylporphine 	CCl_4	$(1.0 \pm 0.3) \times 10^6$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
14.30.1		CCl_4	$k_r = (3.0 \pm 2.1) \times 10^2$		rt	Ad-27	S = ? k_r derived using $k_A = 1.0 \times 10^6$ dm^3 mol^{-1} s^{-1} [*14.30*].	Kras79A010
14.31	mesoporphyrin-IX-dimethyl ester	CCl_4	$(2.5 \pm 0.8) \times 10^6$		rt	Ld-13	S = ? k derived using $k_d = 3.6 \times 10^1$ s^{-1} [*1.8.3*].	Kras79A010
14.32	bilirubin 	D_2O (pD 7)	$k_r = (1.5 \pm 0.4) \times 10^7$ *9.3 $\times 10^6$		rt	Ad-35	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4$ (*3.1 $\times 10^4$) s^{-1} [*1.2.3*].	Math..74F103
14.32.1		D_2O (pD 10)	$k_r = (3.0 \pm 0.7) \times 10^9$ *1.9 $\times 10^9$		rt	Ad-35	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4$ (*3.1 $\times 10^4$) s^{-1} [*1.2.3*].	Math..74F103
14.32.2		MeOH	1.5×10^9		rt	Ad-15	S = RB. k derived using k_d = *1.0 $\times 10^5$ s^{-1} [*1.3.6*].	Ligh.79F104

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

No. Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.32.3	MeOH	$k_r = 2.0 \times 10^8$		rt	Ad-15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.32.4	$CHCl_3$	1.5×10^9	$(6.7 \pm 0.4) \times 10^{-6}$	rt	A'd-16	S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^4$ s^{-1} [*1.5.3*].	Foot.75R071
14.32.5	$CHCl_3$	1.3×10^9	$(7.7 \pm 3.0) \times 10^{-6}$	23	Ad-15	S = MB. k derived using $k_d = *1.0 \times 10^4$ s^{-1} [*1.5.3*].	Foot.75R071
14.32.6	$CHCl_3$	$k_r = 4.3 \times 10^8$ $*2.7 \times 10^8$		rt	Ad-17 P'a	S = MB, A' = TME. Measured ($k_r/k_r^{A'}$) = 9.0 ± 1.4. k_r derived using $k_r^{A'} = 4.8 \times 10^7$ ($*3.0 \times 10^7$) dm^3 mol^{-1} s^{-1} [*2.35.2*].	Foot.75R071
14.32.7	$CHCl_3$	$k_r = 2.1 \times 10^8$ $*1.9 \times 10^8$		rt	Ad-17 A'd	S = MB, A' = DPBF. Measured ($k_r/k_r^{A'}$) = 0.30 ± 0.02. k_r derived using $k_r^{A'} = 7 \times 10^8$ ($*6.3 \times 10^8$) dm^3 mol^{-1} s^{-1} [*5.36.85*].	Foot.75R071
14.32.8	$CHCl_3$	2.8×10^9 $*1.7 \times 10^9$		rt	Ad-15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ ($*1.0 \times 10^4$) s^{-1} [*1.5*].	Ligh.79F104
14.32.9	$CHCl_3$	$k_r = 3.8 \times 10^8$ $*2.3 \times 10^8$		rt	Ad-15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.32.10	CCl_4	$k_r = (1.7 \pm 0.3) \times 10^8$ $k_q = (2.3 \pm 1.0) \times 10^9$		rt	A'd-24	S = A' = Rub. k_r and k_q derived using ($k/k_{A'}$) = 54 ± 0.4, ($k_r/k_{A'}$) = 4 ± 1, and $k_{A'}$ = 4.2×10^7 dm^3 mol^{-1} s^{-1}.	Stev.76R011
14.32.11	CCl_4	$k_r = 1.7 \times 10^8$		rt	A'd-17 Ad	S = A' = Rub. Measured ($k_r/k_r^{A'}$) = 4 ± 1. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.1*].	Stev.76R011
14.32.12	CCl_2F-$CClF_2$	$k_r = (1.0 \pm 0.4) \times 10^7$		rt	Ad-36	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} [*15.1.4*].	Math..74F103
14.32.13	CCl_2F-$CClF_2$	$k_r = (1.0 \pm 0.2) \times 10^8$		rt	Ad-36	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} [*15.1.4*]. Previous value by same workers [74F103] low due to overdepletion of A in solution exposed directly to laser beam.	Math.77F129
14.32.14	C_6H_6	$k_r = 1.7 \times 10^8$		rt	A'd-17 Ad	S = A' = Rub. Measured ($k_r/k_r^{A'}$) = 4 ± 1. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.1*].	Stev.76R011
14.32.15	$CHCl_3$ /MeOH (9:1) v:v	8.4×10^8 (est)	$(3.1 \pm 0.6) \times 10^{-5}$	23	Ad-15	S = RB. k estimated using $k_d = 2.6 \times 10^4$ s^{-1} (calc).	Foot.75R071

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

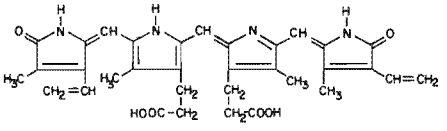
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.32.16		$CHCl_3$ /MeOH (9:1) v:v	$k_r = 2.5 \times 10^8$		rt	Ad-14	S = RB. k_r derived using $\phi_{isc} = 0.66$ and $k_A = 1.5 \times 10^9$ dm^3 mol^{-1} s^{-1} [*14.32.4*].	Foot.75R071
14.33	aetiobilirubin -IVγ	$CHCl_3$	3.0×10^9 *1.8×10^9		rt	Ad-15	S = RBCE. k derived using $k_d = 1.67 \times 10^4$ (*1.0×10^4) s^{-1} [*1.5*].	Ligh.79F104
14.33.1		$CHCl_3$	$k_r = 2.3 \times 10^9$ *1.4×10^9		rt	Ad-15	S = RBCE. k_r derived using $\phi_{isc} = 0.36$.	Ligh.79F104
14.33.2		MeOH /$CHCl_3$ (9:1) v:v	1.6×10^9		rt	Ad-15	S = RB. k derived using k_d = *1.0×10^5 s^{-1} [*1.3.6*].	Ligh.79F104
14.33.3		MeOH /$CHCl_3$ (9:1) v:v	$k_r = 6.2 \times 10^8$		rt	Ad-15	S = RB. k_r derived using $\phi_{isc} = 0.76$.	Ligh.79F104
14.34	biliveridin 	D_2O (pD 8.4)	k_r (3.0 ± 0.1) $\times 10^8$		rt	Ad-35	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4$ s^{-1} and $k_A = 5.1 \times 10^{10}$ dm^3 mol^{-1} s^{-1} [*14.34.1*].	Math.77F129
14.34.1		D_2O (pD 8.4)	$(5.1 \pm 0.4) \times 10^{10}$		rt	A'd-16	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ s^{-1}.	Math.77F129
14.34.2		D_2O (pD 11.8)	$k_r = (4.0 \pm 0.4) \times 10^8$		rt	Ad-35	$^1O_2$* from Nd-YAG CW laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4$ s^{-1} and $k_A = 6.0 \times 10^{10}$ dm^3 mol^{-1} s^{-1} [*14.34.3*].	Math.77F129
14.34.3		D_2O (pD 11.8)	$(6.0 \pm 2.0) \times 10^{10}$		rt	A'd-16	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ s^{-1}.	Math.77F129
14.34.4		D_2O (pD 13.4)	$k_r = (5.1 \pm 1.2) \times 10^8$		rt	Ad-35	$^1O_2$* from Nd-YAG laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4$ s^{-1} and $k_A = 1.5 \times 10^{10}$ dm^3 mol^{-1} s^{-1} [*14.34.5*].	Math.77F129
14.34.5		D_2O (pD 13.4)	$(1.5 \pm 0.3) \times 10^{10}$		rt	A'd-16	$^1O_2$* from Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_d = 5.0 \times 10^4$ s^{-1}.	Math.77F129
14.34.6		$CHCl_3$	$k_r \leqslant 2.9 \times 10^6$		rt	Ad-17 A'd	S = A' = Rub. Measured $(k_r/k_r^{A'}) \leqslant 0.07$. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.1*].	Stev.76R011
14.34.7		$CHCl_3$	2.0×10^9	$(5 \pm 1) \times 10^{-6}$	rt	A'd-23	S = A' = Rub. k derived using k_d = *1.0×10^4 s^{-1} [*1.5.3*].	Stev.76R011

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

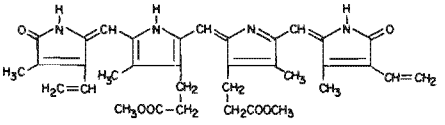
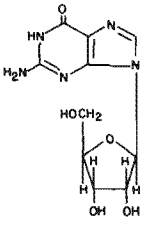
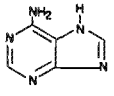
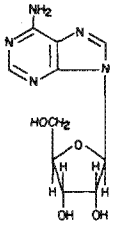
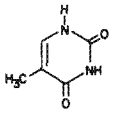
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.35	biliveridin dimethyl ester 	CCl_2F-$CClF_2$	$k_r = (6.0 \pm 0.5) \times 10^5$		rt	A'd-35	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{O_2} = 2.7 \times 10^3$ [*15.1.4*].	Math.77F129
14.35.1		CCl_2F-$CClF_2$	$k_q = (8.0 \pm 2.0) \times 10^8$		rt	A'd-35	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{O_2} = 2.7 \times 10^3$ [*15.1.4*].	Math.77F129
14.35.2		CCl_2F-$CClF_2$	9×10^8		rt	A'd-16	$^1O_2$* from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{O_2} = 2.7 \times 10^3$ dm^3 mol^{-1} s^{-1} [*15.1.4*].	Math.77F129
14.36	guanosine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$		25	Od-19	S = phenosafranine. No measurable effect.	Kral.78A360
14.36.1		H_2O/MeOH (1:1) v:v	$<1\times10^7$		rt	A'd-5	S = MB, A' = DPBF, ruby laser (694 nm).	Nils..72F516
14.37	adenine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$		25	Od-19	S = phenosafranine. No measurable effect.	Kral.78A360
14.38	adenosine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$		25	Od-19	S = phenosafranine. No measurable effect.	Kral.78A360
14.39	thymine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$		25	Od-19	S = phenosafranine. No measurable effect.	Kral.78A360

TABLE 14. Rate constants for the interaction of singlet oxygen with some compounds of biological interest — Continued

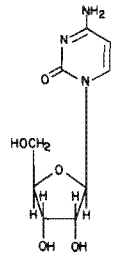
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
14.40	cytidine 	H_2O (pH 7.1)	$\leqslant 1 \times 10^6$		25	Od–19	S = phenosafranine. No measurable effect.	Kral.78A360

TABLE 15. Rate constants for the interaction of singlet oxygen with miscellaneous substrates

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
	[Note: k represents the overall rate constant unless k_r (chemical reaction rate constant) or k_q (quenching rate constant) is specified; k_d is the rate constant for solvent deactivation]							
15.1	oxygen ($^3\Sigma_g^-$) O_2	H_2O (pH 6.2)	5.1×10^2	$(1.15 \pm 0.1) \times 10^{-3}$		A'd-19	S = MB, A' = leuco fluorescein. k derived using k_d = *4.4 × 10^5 s^{-1} [*1.1.3*].	Koiz.68F287
15.1.1		H_2O (pH 6.2)	8.4×10^2	$(1.9 \pm 0.3) \times 10^{-3}$		A'd-19	S = thionine, A'=leuco fluorescein. k derived using k_d = *4.4 × 10^5 s^{-1} [*1.1.3*].	Koiz.68F287
15.1.2		H_2O (pH 6.2)	9.7×10^2	$(2.2 \pm 0.4) \times 10^{-3}$		A'd-19	S = Eos, A' = leuco fluorescein. k derived using k_d = *4.4 × 10^5 s^{-1} [*1.1.3*].	Koiz.68F287
15.1.3		H_2O (pH 6.2)	2.6×10^4	6.0×10^{-2}		A'd-19	S = acridine, A'= leuco fluorescein. k derived using k_d = *4.4 × 10^5 s^{-1} [*1.1.3*].	Koiz.68F287
15.1.4		CCl_2F-$CClF_2$	$(2.7 \pm 0.3) \times 10^3$		rt	A'd-5	$^1O_2$* from pulsed Nd-YAG laser (1065 nm), A' = DPBF.	Math...74F102
15.1.5		C_6H_6	$(6.0 \pm 4.0) \times 10^4$		rt	A'd-?	Reported as unpublished data.	Stev73F659
15.2	methanol CH_3OH	CCl_4	$(3.0 \pm 1.0) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
15.3	ethanol CH_3CH_2OH	CCl_4	$(1.7 \pm 1.1) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
15.4	iodoethane CH_3CH_2I	C_6H_6	2×10^4		rt	A'd-8	S = An, A' = DPBF, ruby laser (347 nm).	Wilk76F902
15.4.1		C_6H_5Br /Me_2CO (2:1) v:v	$\leqslant 10^6$		rt	A'd-23	S = A' = Rub. No measurable effect.	Rose.76F126
15.4.2		C_6H_5Br /MeOH (2:1) v:v	$\leqslant 10^6$		rt	A'd-23	S = A' = Rub. No measurable effect.	Rose.76F126
15.5	2-propanol $CH_3CH(OH)CH_3$	CCl_4	$(1.7 \pm 0.9) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
15.6	1-butanol $CH_3(CH_2)_2CH_2OH$	CCl_4	$(2.4 \pm 0.6) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn..76F903
15.7	2-methyl-2-propanol $(CH_3)_3COH$	CCl_4	$(1.8 \pm 1.5) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn..76F903
15.8	heptane $CH_3(CH_2)_5CH_3$	CCl_4/MeOH (96:4) v:v	$(4 \pm 2) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
15.9	3-methylheptane $CH_3(CH_2)_3CH(CH_3)CH_2CH_3$	CCl_4/MeOH (96:4) v:v	$(5.5 \pm 2.5) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
15.10	4-methylheptane $CH_3(CH_2)_2CH(CH_3)(CH_2)_2CH_3$	CCl_4/MeOH (96:4) v:v	$(5 \pm 2) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, ruby laser (694 nm).	Bort...77F162
15.11	tetrahydrofuran 	CCl_4	$(1.9 \pm 1.1) \times 10^3$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903

COMPOUNDS 15.12 - 15.18 :

TABLE 15. Rate constants for the interaction of singlet oxygen with miscellaneous substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
15.12	2,3-dihydropyran	$(Me)_2CO$	$k_r = 7.2 \times 10^4$ *5.9×10^4		8	?	S = RB, A′ = *p*-dioxene. Measured ($k_r/k_r^{A'}$) = 0.326. k_r derived using $k_r^{A'} = 2.2 \times 10^5$ (*1.8×10^5) dm^3 mol^{-1} s^{-1} [*2.55.1*].	Bart..70F733
15.13	4-methyl-2,3-dihydropyran-2-*t* [R_2 = -T, R_4 = -CH_3]	CH_3CN	$k_r = 6.7 \times 10^4$ (est)		rt	Ad-17 A′d	S = MB, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.067 ± 0.001. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.13.1		C_6H_6	$k_r = 7.3 \times 10^4$ (est)		rt	Ad-17 A′d	S = TPP, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.980 ± 0.010. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.14	4-methyl-2,3-dihydropyran-3-*t* [R_3 = -T, R_4 = -CH_3]	CH_3CN	$k_r = 8.3 \times 10^4$ (est)		rt	Ad-17 A′d	S = TPP, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.866 ± 0.003. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.14.1		C_6H_6	$k_r = 7.9 \times 10^4$ (est)		rt	Ad-17 A′d	S = TPP, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.908 ± 0.006. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.15	4-methyl-2,3-dihydropyran-4-*d* [R_4 = -D, R_4 = -CH_3]	CH_3CN	$k_r = 4.0 \times 10^4$ (est)		rt	?	S = MB, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.787 ± 0.050. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.15.1		C_6H_6	$k_r = 6.6 \times 10^4$ (est)		rt	?	S = TPP, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.087 ± 0.055. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.16	4-methyl-2,3-dihydropyran-4-*t* [R_4 = -T, R_4 = -CH_3]	CH_3CN	$k_r = 5.9 \times 10^4$ (est)		rt	Ad-17 A′d	S = MB, A′ = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.211 ± 0.017. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645

TABLE 15. Rate constants for the interaction of singlet oxygen with miscellaneous substrates — Continued

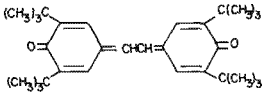
No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
15.16.1		C_6H_6	$k_r = 5.4 \times 10^4$ (est)		rt	Ad-17 A'd	S = TPP, A' = 4-methyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.335 ± 0.023. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.17	4,4-dimethyl-2,3-dihydropyran-2-*t* [R_2 = -T, $R_4 = R_4 = -CH_3$]	CH_3CN	$k_r = 7.2 \times 10^4$ (est)		rt	Ad-17 A'd	S = MB, A' = 4,4-dimethyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 1.001 ± 0.015. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.17.1		C_6H_6	$k_r = 7.2 \times 10^4$ (est)		rt	Ad-17 A'd	S = TPP, A' = 4,4-dimethyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.994 ± 0.007. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.18	4,4-dimethyl-2,3-dihydropyran-3-*t* [R_3 = -T, $R_4 = R_4 = -CH_3$]	CH_3CN	$k_r = 8.0 \times 10^4$ (est)		rt	Ad-17 A'd	S = MB, A' = 4,4-dimethyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.897 ± 0.006. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.18.1		C_6H_6	$k_r = 8.0 \times 10^4$ (est)		rt	Ad-17 A'd	S = TPP, A' = 4,4-dimethyl-2,3-dihydropyran. Measured ($k_r^{A'}/k_r$) = 0.897 ± 0.002. k_r estimated using $k_r^{A'}$ = k_r(2,3-dihydropyran) = 7.2×10^4 dm^3 mol^{-1} s^{-1} [*15.12*].	Frim...77F645
15.19	dioxane 	CCl_4	$(7.0 \pm 15) \times 10^2$		rt	A'd-8	S = MB, A' = DPBF, dye laser (610 nm).	Youn.76F903
15.20	complex diketone-VIII 	CH_2Cl_2	2.3×10^9		30	Od-23	S = MB, A' = 1,3-cyclohexadiene. k derived using $k_{A'}$ = *3.5×10^6 dm^3 mol^{-1} s^{-1} [*A3.8*] and k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Taim.76F921
15.20.1		CH_2Cl_2	4.3×10^9		30	Od-23	S = MB, A' = TME. k derived using $k_{A'}$ = 4.0×10^7 dm^3 mol^{-1} s^{-1} [*2.35.3*] and k_d = *1.2×10^4 s^{-1} [*1.4.2*].	Taim.76F921

TABLE 15. Rate constants for the interaction of singlet oxygen with miscellaneous substrates — Continued

No.	Substrate (A)	Solvent	k /dm^3 mol^{-1} s^{-1}	β (k_d/k) /mol dm^{-3}	t /°C	Method	Comments	Ref.
15.20.2		CH_2Cl_2	5.4×10^9		30	Od-23	S = MB, A′ = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm^3 mol^{-1} s^{-1} [*3.63.3*] and $k_d = *1.2 \times 10^4$ s^{-1} [*1.4.2*].	Taim.76F921
15.21	sodium dodecyl sulfate micelles (SDS)	H_2O	1.0×10^9		40	A′d-23	S = Py, A′ = DPBF, Q = NaN_3. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. S and A′ solubilized in SDS micelles.	Miyo.78A174
15.22	dodecyl trimethyl ammonium chloride micelles (DTAC)	H_2O	1.7×10^8		40	A′d-23	S = Py, A′ = DPBF, Q = NaN_3. k derived using $k_d = 5.0 \times 10^5$ s^{-1} [*1.1*]. S and A′ solubilized in DTAC micelles.	Miyo.78A174
15.23	trimethyl phosphite $(CH_3O)_3P$	Me_2CO	$k_r = 1.6 \times 10^7$		rt	Pa-17 P′a (sep)	S = RB, A′ = triethyl phosphite. Measured $(k_t/k_r^{A'}) = 0.65$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7$ dm^3 mol^{-1} s^{-1} [*15.24*].	Bold.74F495
15.23.1		C_6H_6/MeOH (4:1) v:v	1.52×10^7		rt	Pa-19	S = MB, A′ = Car. k derived using k_d(unreported) and $k_{A'}$(unreported).	Bold.74F495
15.24	triethyl phosphite $(CH_3CH_2O)_3P$	C_6H_6/MeOH (4:1) v:v	2.45×10^7		rt	Pa-19	S = MB, A′ = Car. k derived using k_d(unreported) and $k_{A'}$(unreported).	Bold.74F495
		For more relative rates see		15.25, 15.26.				
15.25	tributyl phosphite $[CH_3(CH_2)_2O]_3P$	Me_2CO	$k_r = 1.9 \times 10^7$		rt	Pa-17 P′a (sep)	S = RB, A′ = triethyl-phosphite. Measured $(k_t/k_r^{A'}) = 0.78$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7$ dm^3 mol^{-1} s^{-1} [*15.24*].	Bold.74F495
15.26	tri*cyclo*hexyl phosphite (*cyclo*-$C_6H_{12}O)_3P$	Me_2CO	$k_r = 1.5 \times 10^7$		rt	Pa-17 P′a (sep)	S = RB, A′ = triethyl-phosphite. Measured $(k_t/k_r^{A'}) = 0.60$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7$ dm^3 mol^{-1} s^{-1} [*15.24*].	Bold.74F495
15.27	triphenyl phosphine $(C_6H_5)_3P$	MeOH	2.0×10^7	5.0×10^{-3}	20	Od-15	S = RB, k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 5.9 kJ mol^{-1}.	Koch68F288
15.27.1		MeOH	1.7×10^7	6.0×10^{-3}	20	Od-15	S = MB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [*1.3.6*]. E_a = 5.0 kJ mol^{-1}.	Koch68F288

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Molecular Formula Index

The molecular formula index is organized according to the number and identity of atoms in a given molecule. Carbon atoms are listed first in a molecular formula followed by hydrogen atoms and an alphabetical listing of the remaining elements of the molecule. In organizing the molecular formulas within the index the formula with the fewest number of carbon atoms is listed first. If two molecular formulas have identical numbers of carbon atoms then the formula with the fewest number of hydrogen atoms is listed first. Molecular formulas with the same number of both carbon and hydrogen atoms are listed in alphabetical order according to the third element in the formula and so forth.

To each *molecular formula* there corresponds a list of compound names. Each compound name has associated with it either entry numbers from tables 1 thru 15 and/or reference numbers (i.e. 79F149) from the Recently Published Results Section.

$C_{17}H_{26}O_3$ Propanoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)-phenyl ester **4.23**

$C_{18}H_{12}$ 1,2-Benzanthracene **3.60**
Naphthacene **3.62**

$C_{18}H_{12}O$ Benzo[b]cyclopentadieno[e]pyran, 2-phenyl- **5.40**

$C_{18}H_{15}P$ Phosphine, triphenyl- **15.27**

$C_{18}H_{16}O$ 2-Penten-1-ol, 3,4,4-trimethyl- **79F137**

$C_{18}H_{16}O_2$ Furfuryl alcohol, α-benzhydryl- **5.15**

$C_{18}H_{18}N_2NiO_2$ Nickel(II), 2,2'-[1,2-ethanediylbis-(nitriloethylidyne)]bis[phenolato(2-)-*N,N',O,O'*]- **10.94**

$C_{18}H_{18}N_4O$ 2-Pyrazolin-5-one, 4-(4'-dimethylamino-phenyl)imino-3-methyl-1-phenyl- **9.18**

$C_{18}H_{20}B_2N_{12}Ni$ Nickel(II), bis[hydrotris(1-pyrazolato)borato]- **10.5**

$C_{18}H_{20}N_2NiO_4$ Nickel(II), bis(2-hydroxy-4-methylacetophenone oximato-*N,O*)- **10.73**

$C_{18}H_{21}NNiO_2S$ Nickel(II), ethaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-*O,O'*]- **10.102**

$C_{18}H_{22}N_2$ Benzene, 1-cyclohexylamino-4-phenylamino- **7.17**

$C_{18}H_{22}N_4Ni$ Nickel(II), bis(1-methylamino-2-methyliminocycloheptatriene-*N,N'*)- **10.46**

$C_{18}H_{23}ClN_2$ Benzene, 1-cyclohexylamino-4-phenylamino-, hydrochloride **7.18**

$C_{18}H_{30}O$ Phenol, 2,4,6-tri(2-methyl-2-propyl)- **4.12**

$C_{18}H_{30}O_2$ Phenol, 4-(2-methyl-2-propoxy)-2,6-di(2-methyl-2-propyl)- **4.13**

$C_{18}H_{33}PO_3$ Phosphite, tricyclohexyl- **15.26**

$C_{18}H_{36}CoN_2S_4$ Cobalt(II), bis(*N,N*-dibutyldithiocarbamato-*S,S'*)- **10.16**

$C_{18}H_{36}CuN_2S_4$ Copper(II), bis(*N,N*-dibutyldithiocarbamato-*S,S'*)- **10.18**

$C_{18}H_{36}N_2NiS_4$ Nickel(II), bis(*N,N*-dibutyldithiocarbamato-*S,S'*)- **10.17**

$C_{18}H_{36}N_2S_4Zn$ Zinc(II), bis(*N,N*-dibutyldithiocarbamato-*S,S'*)- **10.19**

$C_{19}H_{13}O_2S^-$ Fluoren-9-yl anion, 9-benzenesulfonyl **11.47**

$C_{19}H_{22}N_2O_3$ Dregamine **6.31**

$C_{19}H_{32}O_2$ Linolenic acid, methyl ester **14.7**

$C_{19}H_{34}O_2$ Linoleic acid, methyl ester **14.6**

$C_{19}H_{36}O_2$ Oleic acid, methyl ester **14.5**

$C_{19}H_{38}O_2$ Stearic acid, methyl ester **14.4**

$C_{20}H_{14}$ Anthracene, 9-phenyl- **3.51**

$C_{20}H_{14}N_2NiO_2$ Nickel(II), 2,2'-[1,2-phenylenebis-(nitrilomethylidyne)]bis[phenolato(2-)-*N,N',O,O'*]- **10.96**

$C_{20}H_{14}O$ Isobenzofuran, 1,3-diphenyl- **5.36 79A106 79E106 79E611 79E463 79N020 79N041**

$C_{20}H_{16}$ 1,2-Benzanthracene, 9,10-dimethyl- **3.61**

$C_{20}H_{22}N_4O$ 2-Pyrazolin-5-one, 4-(4'-amino-2',3',5',6'-tetramethylphenyl)imino-3-methyl-1-phenyl- **9.17**
2-Pyrazolin-5-one, 4-(4'-diethylaminophenyl)imino-3-methyl-1-phenyl- **9.21**
2-Pyrazolin-5-one, 4-(4'-dimethylamino-3',5'-dimethylphenyl)imino-3-methyl-1-phenyl- **9.19**

$C_{20}H_{24}ClN_3O$ 1,2,3-benzo[2*H*]triazole, 2-[2'-hydroxy-3',5'-di(2-methyl-2- propyl)phenyl]-5-chloro- **4.20**

$C_{20}H_{24}N_2NiO_2$ Nickel(II), bis[2-[(2-propylimino)methyl]phenolato-*N,O*]- **10.78**

$C_{20}H_{25}NNiO_2S$ Nickel(II), butaneamine[2,2'-thiobis(3,4-dimethyl)-phenolato-*O,O'*]- **10.106**

$C_{20}H_{26}N_2O$ Aniline, *N,N*-diethyl-3,5-dimethyl-4-(4'-oxo-2',6'-dimethylcyclohexadienyliden)amino- **9.30**

$C_{20}H_{26}O$ Phenol, 2,6-di(2-methyl-2-propyl)-4-phenyl- **4.14**

$C_{20}H_{28}$ Adamantane, adamantylidene- **2.17**

$C_{20}H_{28}O$ 11-*cis*-Retinal **79F463**
13-*cis*-Retinal **79F463**
Retinal (all *trans*) **79F463**

$C_{20}H_{30}O$ Retinol (all *trans*) **2.119**

$C_{21}H_{19}BrCl_2N_2S_2$ 2,2'-Thiacarbocyanine, 5,5'-dichloro-3,3'-diethyl-, bromide **9.39**

$C_{21}H_{23}IN_2$ 2,2'-Cyanine, 1,1'-diethyl-, iodide **9.34**

$C_{21}H_{24}N_4O$ 2-Pyrazolin-5-one, 4-(4'-diethylamino-2'-methylphenyl)imino-3-methyl-1-phenyl- **9.22**

$C_{21}H_{26}O_3$ Benzophenone, 2-hydroxy-4-octyloxy- **4.3**
Salicylic acid, 4-(1,1,3,3-tetramethylbutyl)phenyl ester **4.2**

$C_{21}H_{28}O$ Phenol, 4-benzyl-2,6-di(2-methyl-2-propyl)- **4.15**

$C_{21}H_{30}O_3$ 7-Dehydroandrosterone-3-acetate **14.16**

$C_{21}H_{32}O_2$ Pregnenolone **14.12**

$C_{21}H_{34}O_2$ Arachidonic acid, methyl ester **14.8**

$C_{21}H_{42}FeN_3S_6$ Iron(III), tris(*N,N*-di-2-propyldithiocarbamato-*S,S'*)- **10.15**

$C_{22}H_{14}$ 1,2,5,6-Dibenzanthracene **3.64**
Pentacene **3.65**

$C_{22}H_{16}N_2O$ Aniline, 4-(2',3'-benzo-4'-oxocyclohexadienyliden)amino-*N*-phenyl- **9.31**

$C_{22}H_{18}O$ Isobenzofuran, 5,6-dimethyl-1,3-diphenyl- **5.37**

$C_{22}H_{26}Br_2N_2NiO_2$ Nickel(II), bis[4-bromo-2-[(butylimino)methyl]-phenolato-*N,O*]- **10.80**

$C_{22}H_{26}N_4O$ 2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'-dimethylphenyl)-imino-3-methyl-1-phenyl- **9.23**
2-Pyrazolin-5-one, 4-(4'-dimethylamino-2',3',5',6'-tetramethylphenyl)imino-3-methyl-1-phenyl- **9.20**

$C_{22}H_{27}NNiO_2S$ Nickel(II), cyclohexaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-*O,O'*]- **10.108**

$C_{22}H_{28}N_2NiO_2$ Nickel(II), bis[2-[(butylimino)methyl]phenolato-*N,O*]- **10.79**
Nickel(II), bis[2-[(1-methylpropylimino)methyl]-phenolato-*N,O*]- **10.82**
Nickel(II), bis[2-[(2-methyl-2-propylimino)methyl]-phenolato-*N,O*]- **10.83**

$C_{22}H_{29}N_3O$ 1,2,3-benzo[2*H*]triazole, 2-[2'-hydroxy-3',5'-di(2-methyl-2-butyl)- phenyl]- **4.21**

$C_{22}H_{32}O_2$ Retinyl acetate **79F463**

$C_{23}H_{21}IN_2S_2$ 2,2'-Thiacarbocyanine, 3,8,3',10-di(1,3-propanediyl)-, iodide **9.51**

$C_{23}H_{23}BrCl_2N_2S_2$ 2,2'-Thiacarbocyanine, 5,5'-dichloro-3,9,3'-triethyl-, bromide **9.44**

$C_{23}H_{23}IN_2S_2$ 2,2'-Thiadicarbocyanine, 3,3'-diethyl-, iodide **9.52**

$C_{23}H_{25}BrN_2S_2$ 2,2'-Thiacarbocyanine, 3,9,3'-triethyl-, bromide **9.42**

$C_{23}H_{29}N_3O_2$ Aniline, *N,N*-diethyl-4-[*N*-(phenylaminocarbonyl)-pivaloylmethylene]amino- **9.10**

$C_{23}H_{32}O_3$ 16-Dehydropregnenolone-3-acetate **14.15**

$C_{24}H_{36}N_2O_2$ Aniline, 4-(*N*-dipivaloylmethylene)amino-3,*N,N*-triethyl- **9.7**

$C_{24}H_{16}N_2NiO_2$ Nickel(II), 2,2-[1,8-naphthalenediylbis-(nitrilomethylidyne)]bis[phenolato(2-)-*N,N',O,O'*]- **10.97**

$C_{24}H_{18}O$ Phenol, 2,4,6-triphenyl- **4.22**

$C_{24}H_{20}$ 2-Butene, 2,3-di(α-naphthyl)- **79F051**

$C_{24}H_{20}$ 2-Butene, 2,3-di(β-naphthyl)- **79F051**

$C_{24}H_{20}CoO_4P_2S_4$ Cobalt(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.28**

$C_{24}H_{20}CrO_4P_2S_4$ Chromium(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.32**

$C_{24}H_{20}CuO_4P_2S_4$ Copper(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.30**

$C_{24}H_{20}NiO_4P_2S_4$ Nickel(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.29**

$C_{24}H_{20}O_4P_2PbS_4$ Lead(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.33**

$C_{24}H_{20}O_4P_2S_4Zn$ Zinc(II), bis(*O,O'*-diphenyldithiophosphato-*S,S'*)- **10.31**

$C_{24}H_{25}IN_2S_2$ 2,2'-Thiacarbocyanine, 3,3'-diethyl-8,9-(1,3-propanediyl)-, iodide **9.50**

$C_{24}H_{30}N_4O$ 2-Pyrazolin-5-one, 4-(4'-diethylamino-2'-methylphenyl)imino-3-(2-methyl-2-propyl)-1-phenyl- **9.24**

$C_{24}H_{31}N_3O_2$ Aniline, *N,N*-diethyl-3-methyl-4-[*N*-(phenylamino-carbonyl)pivaloylmethylene]amino- **9.11**

$C_{24}H_{32}N_2NiO_4$ Nickel(II), bis[2-[(butylimino)methyl]-4-methoxy-phenolato-*N,O*]- **10.81**

$C_{24}H_{44}CoO_4P_2S_4$ Cobalt(II), bis(*O,O'*-dicyclohexyldithiophosphato-*S,S'*)- **10.26**

$C_{24}H_{44}NiP_2S_4$ Nickel(II), bis(dicyclohexyldithiophosphinato-*S,S'*)- **10.27**

$C_{25}H_{19}N$ 4-*H*-Cyclopentadieno[b]quinoline, 1,2-diphenyl-4-methyl- **5.46**

$C_{25}H_{23}BF_4N_4S_2$ 2,2'-Thiacarbocyanine, 5,5'-dicyano-3,9,3'-triethyl-, tetrafluoroborate **9.45**

$C_{25}H_{25}ClN_2$ 2,2'-Carbocyanine, 1,1'-diethyl-, chloride **9.36**

$C_{25}H_{25}IN_2S_2$ 2,2'-Thiatricarbocyanine, 3,3'-diethyl-, iodide **9.53**

$C_{25}H_{25}N_3O_2$ Aniline, 4-[*N*-benzoyl(phenylaminocarbonyl)-methylene]amino-*N*,*N*-diethyl- **9.12**

$C_{25}H_{26}N_4O_2$ Aniline, 4-[*N*-di(phenylaminocarbonyl)methylene]-amino-*N*,*N*-diethyl- **9.15**

$C_{25}H_{32}N_4O$ 2-Pyrazolin-5-one, 4-(4′-diethylamino-2′,6′-dimethylphenyl)-imino-3-(2-methyl-2-propyl)-1-phenyl- **9.25**

$C_{25}H_{34}O_3$ Benzophenone, 2-hydroxy-4-dodecyloxy- **4.4**

$C_{26}H_{16}$ 9,9′-Bifluorenylidene **3.43**

$C_{26}H_{17}Cl$ Anthracene, 1-chloro-9,10-diphenyl- **3.57**

$C_{26}H_{18}$ Anthracene, 9,10-diphenyl- **3.56**

$C_{26}H_{20}CoN_2O_2$ Cobalt(II), bis[2-[(phenylimino)methyl]phenolato-*N*,*O*]- **10.85**

$C_{26}H_{20}CuN_2O_2$ Copper(II), bis[2-[(phenylimino)methyl]phenolato-*N*,*O*]- **10.87**

$C_{26}H_{20}N_2NiO_2$ Nickel(II), bis[2-[(phenylimino)methyl]phenolato-*N*,*O*]- **10.86**

$C_{26}H_{20}N_2NiS_4$ Nickel(II), bis(*N*,*N*-diphenyldithiocarbamato-*S*,*S*′)- **10.20**

$C_{26}H_{22}N_4NiO_2$ Nickel(II), bis[2-[(4-aminophenylimino)methyl]-phenolato-*N*,*O*]- **10.91**

Nickel(II), bis[2-(phenylaminoimino)methylphenolato-*N*,*O*]- **10.77**

$C_{26}H_{27}N_3O_2$ Aniline, 4-[*N*-benzoyl(phenylaminocarbonyl)-methylene]amino-*N*,*N*-diethyl-3-methyl- **9.13**

$C_{26}H_{32}N_2NiO_2$ Nickel(II), bis[2-[(cyclohexylimino)methyl]phenolato-*N*,*O*]- **10.84**

$C_{26}H_{34}CoO_4$ Cobalt(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato-*O*,*O*′]- **10.69**

$C_{26}H_{34}NiO_4$ Nickel(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato-*O*,*O*′]- **10.70**

$C_{27}H_{21}N$ Anthracene, 1-methylamino-9,10-diphenyl- **3.58**

$C_{27}H_{23}ClN_2S_2$ 4,5,4′,5′-Dibenzo-2,2′-thiacyanine, 3,3′-diethyl-, chloride **9.35**

$C_{27}H_{26}N_2O_3S_3$ 2,2′-Thiacarbocyanine, 3,3′-diethyl-, toluenesulfonate **9.37**

$C_{27}H_{28}N_2O_2$ Aniline, 4-(dibenzoylmethylene)amino-3,*N*,*N*-triethyl- **9.8**

$C_{27}H_{29}N_3O_2$ Aniline, 4-[*N*-benzoyl(phenylaminocarbonyl)-methylene]amino-3,5-dimethyl-*N*,*N*-diethyl- **9.14**

$C_{27}H_{30}N_4O_2$ Aniline, 4-[*N*-di(phenylaminocarbonyl)methylene]-amino-3-*N*,*N*-triethyl- **9.9**

$C_{27}H_{46}O$ Cholesterol **14.9**

$C_{27}H_{46}O_2$ δ-Tocopherol **4.25**

$C_{28}H_{14}O_2$ 1,2,7,8-Dibenzperylene-3,9-quinone **3.66**

$C_{28}H_{20}N_2O$ Aniline, 4-(2′,3′-benzo-4′-oxocyclohexa-dienylidene)amino-*N*,*N*-diphenyl- **9.32**

$C_{28}H_{20}NiS_4^{2-}$ Nickelate(II) ion, bis(1,2-diphenylethanedithionato(2-)-*S*,*S*′)- **10.50**

$C_{28}H_{20}O$ Furan, 2,3,4,5-tetraphenyl- **5.33 79A106**

$C_{28}H_{20}O_2$ *p*-Dioxin, tetraphenyl- **79A241**

$C_{28}H_{22}N_4O$ 2-Pyrazolin-5-one, 4-(4′-diphenylaminophenyl)imino-3-methyl-1-phenyl- **9.27**

$C_{28}H_{22}NiO_4$ Nickel(II), bis(2-hydroxy-5-methylbenzophenonato-*O*,*O*′)- **10.63**

$C_{28}H_{22}O_2$ Anthracene, 1,4-dimethoxy-9,10-diphenyl- **3.59**

$C_{28}H_{28}CoO_4P_2S_4$ Cobalt(II), bis(*O*,*O*′-di-4-methylphenyldithio-phosphato-*S*,*S*′)- **10.37**

$C_{28}H_{28}CuO_4P_2S_4$ Copper(II), bis(*O*,*O*′-di-4-methylphenyldithio-phosphato-*S*,*S*′)- **10.39**

$C_{28}H_{28}NiO_4P_2S_4$ Nickel(II), bis(*O*,*O*′-di-4-methylphenyldithio-phosphato-*S*,*S*′)- **10.38**

$C_{28}H_{29}N_5O_2$ 2-Pyrazolin-5-one, 4-(4′-diethylamino-2′,6′-dimethylphenyl)-imino-3-(benzoylamino)-1-phenyl- **9.26**

$C_{28}H_{40}NiO_2S$ Nickel(II), bis[2,2′-thiobis-4-(1,1,3,3-tetramethyl-butyl)phenolato-*O*,*O*′]- **10.114**

$C_{28}H_{41}NNiO_2S$ Nickel(II), dodecaneamine[2,2′-thiobis(3,4-dimethyl)-phenolato-*O*,*O*′]- **10.111**

$C_{28}H_{42}NiO_3S$ Nickel(II), aqua[2,2′-thiobis-4-(1,1,3,3-tetramethyl-butyl)phenolato-*O*,*O*]- **10.98**

$C_{28}H_{42}O_2S$ Phenol, 2,2′-thiobis[4-(1,1,3,3-tetramethyl-butyl)-**4.32**

$C_{28}H_{43}N$ Diphenylamine, 4,4′-di(1,1,3,3-tetramethylbutyl)- **7.5**

$C_{28}H_{43}NNiO_2S$ Nickel(II), ammine[2,2′-thiobis-4-(1,1,3,3-tetra-methylbutyl)phenolato-*O*,*O*′]- **10.100**

$C_{28}H_{44}O$ Ergosterol **14.11**

$C_{28}H_{48}O_2$ β-Tocopherol **4.26**

γ-Tocopherol **4.27**

$C_{29}H_{20}O$ Cyclopentadienone, tetraphenyl- **3.38**

$C_{29}H_{28}N_2O_3S_3$ 2,2′-Thiacarbocyanine, 3,3′-diethyl-8,10-ethanediyl-, toluenesulfonate **9.49**

$C_{29}H_{30}N_2O_3S_3$ 2,2′-Thiacarbocyanine, 3,3′-diethyl-8,10-dimethyl-, toluenesulfonate **9.47**

$C_{29}H_{30}N_2O_5S_3$ 2,2′-Thiacarbocyanine, 3,3′-diethyl-5,5′-dimethoxy-, toluenesulfonate **9.38**

$C_{29}H_{42}O_3$ Benzoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)-, 2′,4′-di(2-methyl-2-propyl)phenyl ester **4.18**

$C_{29}H_{50}O_2$ α-Tocopherol **4.28**

$C_{30}H_{24}Cl_2N_6Ru$ Ruthenium(II), tris(2,2′-bipyridine)-, dichloride **10.45**

$C_{30}H_{28}N_6O_2$ 2-Pyrazolin-5-one, 4,4′-[2,3,5,6-tetramethyl-phenylenebis]-3-methyl-1-phenyl- **9.29**

$C_{30}H_{30}FN_3O_5$ Aniline, 4-[2′,3′-benzo-4′-oxo-5′-(2-methoxy-5-fluorosulfonylphenyl)amino-*N*,*N*′-diphenyl- **9.33**

$C_{30}H_{40}O$ β-8′-Carotenal (*apo*) **2.125**

$C_{30}H_{42}O$ β-8′-Carotenol (*apo*) **2.126**

$C_{30}H_{42}O_2$ 2,5-Cyclohexadien-4-one, 1,2-ethanediylidenebis[3,5-di(2-methyl-2-propyl)- **15.20**

$C_{30}H_{44}$ Carotene analog, C-30 **2.121**

$C_{30}H_{45}NNiO_2S$ Nickel(II), ethaneamine[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.101**

$C_{30}H_{48}CoN_2S_4$ Cobaltate(II), bis[toluene-3,4-dithiolato(2-)-*S*,*S*′]-, di(tetrabutylammonium) **10.51**

$C_{30}H_{48}N_2NiS_4$ Nickelate(II), bis[toluene-3,4-dithiolato(2-)-*S*,*S*′]-, di(tetrabutylammonium) **10.52**

$C_{31}H_{29}BrN_2S_2$ 4,5,4′,5′-Dibenzo-2,2′-thiacarbocyanine, 3,9,3′-triethyl-, bromide **9.46**

$C_{31}H_{30}N_2O_3S$ 4,4′-Carbocyanine, 1,1′-diethyl-, toluenesulfonate **9.41**

$C_{31}H_{32}IN_3$ 2,2′-Carbocyanine, 1,3,3,1′,3′,3′-hexamethyl-8,10-indolo-, iodide **9.48**

$C_{31}H_{34}N_2O_5S_3$ 2,2′-Thiacarbocyanine, 3,9,3 -triethyl-5,5′-dimethoxy-, toluenesulfonate **9.43**

$C_{31}H_{47}NNiO_2S$ Nickel(II), propaneamine[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.103**

$C_{31}H_{50}O_2$ Stigmasteryl acetate **14.13**

$C_{31}H_{52}O_2$ Sitosteryl acetate **14.14**

$C_{31}H_{52}O_3$ α-Tocopheryl acetate **14.3**

$C_{32}H_{22}O$ Isobenzofuran, 1,3,4,7-tetraphenyl- **5.38**

$C_{32}H_{44}O_2$ β-8′-Carotenoic acid, ethyl ester (*apo*) **2.127**

$C_{32}H_{49}CoNO_2S$ Cobalt(II), butaneamine[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.104**

$C_{32}H_{49}NNiO_2S$ Nickel(II), butaneamine[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.105**

$C_{33}H_{34}N_4O_6$ Biliverdine **14.34**

$C_{33}H_{36}N_4O_6$ Bilirubin **14.32 79A111**

$C_{34}H_{34}NiO_6$ Nickel(II), bis[2-hydroxy-4-(2-methyl-2-propyl)-phenylbenzoato-*O*,*O*′]- **10.68**

$C_{34}H_{45}NNiO_2S$ Nickel(II), benzeneamine[2,2′-thiobis-4-(1,1,3,3-tetramethyl)phenolato-*O*,*O*′]- **10.109**

$C_{34}H_{50}N_2NiO_2$ Nickel(II), 2,2′-[1,2-ethanediylbis(nitrilo-decylidene)]bis[4-methylphenolato(2-)-*N*,*N*′,*O*,*O*′]- **10.95**

$C_{34}H_{50}O_2$ Cholesteryl benzoate **14.10**

$C_{34}H_{51}NNiO_2S$ Nickel(II), cyclohexaneamine[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.107**

$C_{34}H_{53}NNiO_5S$ Nickel(II), nitrilotris(2-hydroxyethyl)[2,2′-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-*O*,*O*′]- **10.113**

$C_{34}H_{56}NiO_8P_2$ Nickel(II), bis[*O*-ethyl-[3,5-di-(2-methyl-2-propyl)-4-hydroxybenzyl]phosphonato-*O*,*O*′]- **10.22**

$C_{35}H_{30}N_2O_3S_3$ 4,5,4′,5′-Dibenzo-2,2′-thiacarbocyanine, 3,3′-diethyl-, toluenesulfonate **9.40**

$C_{35}H_{38}N_4O_6$ Biliverdine dimethyl ester **14.35**

Compound Name Index

The compound name index is organized alphabetically according to compound name. Each name is followed immediately by either entry numbers from tables 1 thru 15 and/or reference numbers (i.e. 79F314) from the Recently Published Reference Section.

Styrene, *p*-methyl-α,β,β-trimethyl- **3.13**
Styrene, α,β,β-trimethyl- **3.10**
Sulfate, dodecyl sodium, micelles (SDS) **15.21**
Sulfide, benzyl methyl **11.5**
Sulfide, 4-bromophenyl methyl **11.9**
Sulfide, butyl methyl **11.3**
Sulfide, 2-butyl 1-propyl **11.18**
Sulfide, 3-chlorophenyl methyl **11.7**
Sulfide, 4-chlorophenyl methyl **11.8**
Sulfide, dibenzyl **11.24**
Sulfide, dibutyl **11.20**
Sulfide, di-(2-butyl) **11.21**
Sulfide, diethyl **11.14**
Sulfide, 2,2′-dihydroxydiethyl **11.16**
Sulfide, diisopropyl **11.17**
Sulfide, di-(2-methyl-2-propyl) **11.22**
Sulfide, diphenyl **11.23**
Sulfide, ethyl 2-methyl-2-propyl **11.15**
Sulfide, 4-fluorophenyl methyl **11.6**
Sulfide, 4-methoxyphenyl methyl **11.12**
Sulfide, methyl 3-methylphenyl **11.10**
Sulfide, *methyl 4-methylphenyl* **11.11**
Sulfide, methyl 4-(2-methyl-2-propyl)phenyl **11.13**
Sulfide, methyl phenyl **11.4**
Sulfide, 2-methyl-2-propyl 1-propyl **11.19**
Sulfoxide, dimethyl- **1a.1**
Superoxide dismutase **8.9**
Superoxide ion **12.10 12.11**
α-Terpinene **2.92**
Terpinolene **2.61**
Tetracene **3.62**
Tetracyclone **5.33**
Tetramethylethylene **2.35**
Tetramethylethylene-d_6 **79F155**
2,2′-Thiacarbocyanine, 5,5′-dichloro-3,3′-diethyl-, bromide **9.39**
2,2′-Thiacarbocyanine, 5,5′-dichloro-3,9,3′-triethyl-, bromide **9.44**
2,2′-Thiacarbocyanine, 5,5′-dicyano-3,9,3′-triethyl-, tetrafluoroborate **9.45**
2,2′-Thiacarbocyanine, 3,3′-diethyl-, toluenesulfonate **9.37**
2,2′-Thiacarbocyanine, 3,3′-diethyl-5,5′-dimethoxy-, toluenesulfonate **9.38**
2,2′-Thiacarbocyanine, 3,3′-diethyl-8,10-dimethyl-, toluenesulfonate **9.47**
2,2′-Thiacarbocyanine, 3,3′-diethyl-8,10-ethanediyl-, toluenesulfonate **9.49**
2,2′-Thiacarbocyanine, 3,3′-diethyl-8,9-(1,3-propanediyl)-, iodide **9.50**
2,2′-Thiacarbocyanine, 3,8,3′,10-di(1,3-propanediyl)-, iodide **9.51**
2,2′-Thiacarbocyanine, 3,9,3′-triethyl-, bromide **9.42**
2,2′-Thiacarbocyanine, 3,9,3′-triethyl-5,5′-dimethoxy-, toluenesulfonate **9.43**
Thiacycloheptane **11.28**
Thiacyclohexane **11.26**
2,2′-Thiadicarbocyanine, 3,3′-diethyl-, iodide **9.52**
2,2′-Thiatricarbocyanine, 3,3′-diethyl-, iodide **9.53**
Thiepane **11.28**
Thiophene **11.35**
Thiophene, tetrahydro- **11.25**
Thiopyran, tetrahydro- **11.26**
4*H*-Thiopyran-4-thione **11.43**
4*H*-Thiopyran-4-thione, 2,6-diphenyl- **11.44**
Thiourea **11.29**
Thiourea, *N*-allyl- **11.31**
Thiourea, *N*-methyl- **11.30**
Thymine **14.39**
α-Tocopherol **4.28 79F463**
β-Tocopherol **4.26**
γ-Tocopherol **4.27**
δ-Tocopherol **4.25**
α-Tocopheryl acetate **14.3**
Toluene **1.36 79E699**
4*H*-[1,2,4]Triazolo[1,2,a]norbornane, 4-methyl-3,5-dioxo- **5.50a**
Tributylamine **6.28**
Triethylamine **6.23**
Trimethylamine **6.22**
Trypsin **8.13**
Tryptophan **79A112 8.8**
Tyramine **8.6**
Tyrosine **79A112 8.5**
1,6-Undecadiene, 2,6-dimethyl- (*cis*) **2.110**
1,6-Undecadiene, 2,6-dimethyl- (*trans*) **2.109**
Urea, *N*-allyl- **6.37**
Vitamin E acetate **14.3**
Water **1.1 1.38 1.48 79N041**
Water-d_2 **1.2 1.39 1a.8 79A111 79N041**
Zinc(II), bis(*N*,*N*-dibutyldithiocarbamato-*S*,*S*′)- **10.19**
Zinc(II), bis(*O*,*O*′-diphenyldithiophosphato-*S*,*S*′)- **10.31**
Zinc(II), bis(*N*,*N*-di-2-propyldithiocarbamato-*S*,*S*′)- **10.14**
Zinc(II), bis(2,4-pentanedionato-*O*,*O*′)- **10.57**
Zinc(II), bis[2,2′-thiobis[*O*,*O*′-di-4-(2-methyl-2-propyl)phenyl]-dithiophosphato-*S*,*S*′]- **10.42**
Zinc(II), tetraphenylchlorinato- **10.122**
Zinc(II), tetraphenylporphinato- **10.119**

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1,3-diphenylisobenzofuran
2,5-dimethylfuran
2,3,4,5-tetraphenylfuran
2,5-di-*t*-butylfuran
2,5-*diphenylfuran*
2,3-diphenylfuran
2,5-di(*p*-chlorophenyl)furan
cyclopentadiene
furan
2,3-dimethylindole
3-methyl-2-phenylindole
3-methylindole
indole

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bilirubin
k_d-H_2O

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histidine
tryptophan
methionine
tyrosine
alanine

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$O_2(^3\Sigma_g)$
1,3-diphenylisobenzofuran
5′-oxo-4-ethyl-3′-ethylidene-3,5,4′-trimethyl-1′,5′-dihydro(2.2′)dipyrromethene
5′-oxo-4-ethyl-3,5-dimethyl-1′,5′-dihydro-(2.2′)dipyrromethene
5′-oxo-3′-ethyl-4′, 5′-dimethyl-1′,5′-dihydro(2,2′)-dipyrromethene

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tetraphenyl-*p*-dioxin

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1,3-diphenylisobenzofuran

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1,3-diphenylisobenzofuran

79E699 Byteva, I.M., Gurinovitch, G.P., Sensitized luminescence of oxygen solutions, J. Lumin. **21**: 17-20 (1979).

k_d-CCl_4
k_d-$CHCl_3$
k_d-C_6H_6
k_d-$C_6H_5CH_3$
k_d-$(CH_3)_2CO$
k_d-C_5H_5N
k_d-$(CH_3CH_2)_2O$
k_d-CH_3CH_2OH

79F051 Adam, W., Carballeira, N., Cheng, C.-C., Sakanishi, K., Gleiter, R., Differentiation in singlet oxygenation rates of 2,3-diaryl-2-butenes as a function of cis-trans isomerism, J. Org. Chem. **44**(5): 851-3 (1979).

cis-2,3-diphenyl-2-butene
trans-2,3-diphenyl-2-butene
cis-2,3-di-β-naphthyl-2-butene
trans-2,3-di-β-naphthyl-2-butene
cis-2,3-di-α-naphthyl-2-butene
trans-2,3-di-α-naphthyl-2-butene

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4,4′-diethyl-3,5,3′,5′-tetramethyldipyrromethane
4,4′-diethyl-3,5,5′,5′-tetramethyldipyrromethene

79F119 Frimer, A.A., Farkash, T., Sprecher, M., Effect of strain on singlet oxygen ($^1O_2$) reactions. 2. Photooxidation of methylenecyclopropanes, J. Org. Chem. **44**(6): 989-95 (1979).

isopropylidenecyclopropane
cyclopropylidenedicyclopropylmethane

79F137 Schulte-Elte, K.H., Muller, B.L., Pamingle, H., Photooxygenation of 3,3-dialkylsubstituted allyl alcohols. Occurrence of syn preference in the ene addition of $^1O_2$ at E/Z-isomeric allyl alcohols, Helv. Chim. Acta **62**(3): 816-29 (1979).

3-methyl-2-butenol
3-ethyl-2-pentenol
2-cyclopentylidene-ethanol
2-cyclohexylidene-ethanol
2-cyclooctylidene-ethanol
2-cyclododecylidene-ethanol
(E)-3-methyl-2-pentenol
(Z)-3-methyl-2-pentenol
(E)-3,7-dimethylocta-2,7-dienol
(Z)-3,7-dimethylocta-2,7-dienol
(E)-3,4-dimethyl-2-octenol
(Z)-3,4-dimethyl-2-octenol
(E)-3,4-dimethyl-2-pentenol
(Z)-3,4-dimethyl-2-pentenol
(E)-3,4,4-trimethyl-2-pentenol
(Z)-3,4,4-trimethyl-2-pentenol

79F148 Stevens, B., Kaplan, S.J., The photoperoxidation of unsaturated organic molecules. XVIII. Malachite green and leucomalachite green, Mol. Photochem. **9**(2): 205-11 (1979).

Malachite Green
Leucomalachite Green
9,10-dimethylanthracene

79F155 Grdina, B., Orfanopoulos, M., Stephenson, L.M., Stereochemical dependence of isotope effects in the singlet oxygen-olefin reaction, J. Am. Chem. Soc. **101**(11): 3111-2 (1979).

cis-tetramethylethylene-d_6
trans-tetramethylethylene-d_6
2-methyl-2-pentene-4*d*

79F268 Lucki, J., Rabek, J.F., Ranby, B., Stabilizing effect of 4-(1-imidazolyl)-phenol against the oxidation of polybutadiene by molecular and singlet oxygen, Polym. Bull. **1**(8): 563-8 (1979).

4-(1-imidazolyl)-phenol

79F278 Landis, M.E., Madoux, D.C., Photooxidatiion of azines. Evidence for a free-radical oxidation initiated by singlet oxygen, J. Am. Chem. Soc. **101**(17): 5106-7 (1979).

acetone azine
tetramethyl-4*H*-pyrazole

79F314 de Mol, N.J., Beijersbergen van Henegouwen, G.M.J., Formation of singlet molecular oxygen by 8-methoxypsoralen, Photochem. Photobiol. **30**(3): 331-5 (1979).

3,4-dihydroxyphenylalanine

79F315 Cornelissen, P.J.G., Beijersbergen van Henegouwen, G.M.J., Photochemical decomposition of 1,4-benzodiazepines Nitrazepam, Photochem. Photobiol. **30**(3): 337-41 (1979).

3,4-dihydroxyphenylalanine

79F463 Krasnovsky, A.A., Kagan, V.E., Photosensitization and quenching of singlet oxygen by pigments and lipids of photoreceptor cells of the retina, FEBS Lett **108**(1): 152-4 (1979).

DABCO
1,3-diphenylisobenzofuran
β-carotene
α-tocopherol
all *trans*-retinal
11-*cis*-retinal
13-*cis*-retinal
retinyl acetate

79N020 Miyoshi, N., Tomita, G., Quenching of singlet oxygen by sodium azide in reversed micellar systems, Z. Naturforsch., Teil B **34B**(2): 339-43 (1979).

1,3-diphenylisobenzofuran
N_3^- in dodecylammonium propionate micelles

79N041 Lindig, B.A., Rodgers, M.A.J., Laser photolysis studies of singlet molecular oxygen in aqueous micellar dispersions, J. Phys. Chem. **83**(13): 1683-8 (1979).

k_d-H_2O(micelles)
k_d-D_2O(micelles)
1,3-diphenylisobenzofuran(micelles)

Appendix I

A More Complete Kinetic Scheme

In the kinetic scheme shown in figure 1, S = Sensitizer, $^1S^*$ = Excited singlet state, $^3S^*$ = Excited triplet state, A = Reactive substrate, and Q = Quencher. Elementary reactions labeled with first order, or psuedo first order rate constants in the case of bimolecular steps, are listed below.

Elementary Reaction	Process	Rate Constant
$^1S + h\nu \rightarrow {}^1S^*$	Absorption (Rate = I_a)	
$^1S^* \rightarrow {}^1S_0 + h\nu$	Fluroescence of $^1S^*$	k_F
$^1S^* \rightarrow {}^1S_0$	Radiationless decay of $^1S^*$	k_{Sd}
$^1S^* + Q \rightarrow {}^1S_0 + Q$	Quenching of $^1S^*$ by Q	k_{Sd}^Q
$^1S^* + {}^3O_2 \rightarrow$ products	Reaction of $^1S^*$ with O_2	k_{Sr}^{O2}
$^1S^* + A \rightarrow$ products	Reaction of $^1S^*$ with A	k_{Sr}^A
$^1S^* \rightarrow {}^3S^*$	Intersystem Crossing from $^1S^*$	k_{isc}
$^1S^* + Q \rightarrow {}^3S^* + Q$	Catalyzed intersystem crossing by Q	k_{isc}^Q
$^1S^* + {}^3O_2 \rightarrow {}^3S^* + {}^3O_2$	Catalyzed intersystem crossing by O_2.	k_{isc}^{O2}
$^1S^* + {}^3O_2 \rightarrow {}^3S^* + {}^1O_2^*$	Energy transfer from $^1S^*$ to give $^1O_2^*$ and $^3S^*$	$k_{S\Delta}^{O2}$
$^3S^* \rightarrow {}^1S$	Decay of $^3S^*$	k_{Td}
$^3S^* + Q \rightarrow {}^1S + Q$	Catalyzed triplet decay by Q	k_{Td}^Q
$^3S^* + {}^3O_2 \rightarrow {}^1S + {}^3O_2$	Catalyzed triplet decay by O_2	k_{Td}^{O2}
$^3S^* + {}^3O_2 \rightarrow$ *products*	Reactions of $^3S^*$ *with* O_2	k_{Tr}^{O2}
$^3S^* + A \rightarrow$ products	Reaction to $^3S^*$ with A	k_{Tr}^A
$^3S^* + {}^3O_2 \rightarrow {}^1S + {}^1O_2^*$	Energy transfer from $^3S^*$ to give $^1O_2^*$	$k_{T\Delta}^{O2}$
$^1O_2^* \rightarrow {}^3O_2$	Decay of singlet oxygen	k_d
$^1O_2^* + A \rightarrow$ products	Reaction of $^1O_2^*$ with A	k_r^A
$^1O_2^* + A \rightarrow {}^3O_2 + A$	Physical Quenching of $^1O_2^*$ by A	k_q^A
$^1O_2^* + Q \rightarrow {}^3O_2 + Q$	Physical Quenching of $^1O_2^*$ by Q	k_q^Q
$^1O_2^* + Q \rightarrow$ products	Reaction of $^1O_2^*$ with Q	k_r^Q

Appendix II

Global Adjustment of Second Order Rate Constants[2]

The purpose of the global adjustment is to obtain better values of the rate constants k_r by ignoring solvent effects and thereby increasing the number of measurements applicable to each value. The premise is that the scatter in the data is greater than the effect of the solvent. Water is a possible exception which, as a solvent, does seem to be associated with larger rate constant values. Included in the effort are all of the interrelations due to many measurements of one value relative to another so that selecting one value affects several others.

The values of k_r for differing compounds range over six orders of magnitude, thus the global adjustment of best values, $\langle k_r \rangle$, requires a measure of best fit insensitive to this range. Further, the scatter in the data is such that two measurements of the same quantity may differ by as much as one order of magnitude without our knowing which is the more nearly correct. For the former reason we choose to adjust values so that $(k_r/\langle k_r \rangle)$should approach 1.0. For the latter reason we measure the deviation from 1.0 as $\log_{10}(k_r/\langle k_r \rangle)$. Thus $(k_r/\langle k_r \rangle) = 1/2$ is considered to be as much too small as $(k_r/\langle k_r \rangle) = 2.0$ is too large.

For the purposes of global adjustment it is assumed that the best estimates for the rate constants, $\langle k_r \rangle$, will be those which minimize the sum of squares of the above deviations, the sum being carried out over all measurements. Implicit in this is the assignment of equal weights to all measurements, which is to say that we act as if each measurement is as valid as any other measurement. Thus the expected error is the same without regard to who made the measurement, what the solvent was, what the substance was or what technique was used.

As a starting point for the adjustment, tables 2 through 15 were scanned for appropriate data. A compound was selected if the comments column indicated that one or more of the measurements was relative to another compound and gives a numerical value for the ratio $(k_r/k_r^{A'})$ or its inverse. It is further required, either that ratios are given for two or more reference compounds, A', or that a value is determined for k_r which is independent of reference compounds. That is, only those compounds are included which can change the value of k_r for another compound when a global fitting for best values is attempted. To this list is added any compound used as a reference but not otherwise included. Excluded from this list are a few measurements which are ratios of rates, but for which only a final value of the rate constant is given but not the value of the ratio. Several values of total quenching rate constant, k_A, are taken as the reactive component, k_r^A, for olefins, aromatics and furans, but carotenes are not included since it is known that physical quenching is dominant. The resulting list contains almost 500 measurements, on 59 compounds measured in about 40 different solvents.

[2]The statistical analysis outlined in this appendix was developed by Dr. W. Phillip Helman of the Radiation Chemistry Data Center.

The data are tabulated by compound, solvent, data type and reference substance where appropriate. The solvents are in some cases mixed which is indicated either by X for MeOH/*t*-BuOH (1:1) (v:v), or by Y for other mixed solvents. The compound and reference are identified by table number, e.g. 2.1 for ethoxyethene.

The values $\langle k_r \rangle$ for each compound were adjusted to minimize the sum of the squares of deviations $(\Sigma'[\ln(k_r^A) - \ln(\langle k_r^A \rangle)]^2 + \Sigma''[\ln(R) - \ln(\langle k_r^A \rangle) + \ln(\langle k_r^{A'} \rangle)]^2)$ without regard to solvent. The sum consists of two parts, Σ' is a sum over all directly determined rate data, Σ'' is the sum of data determined as a ratio of rate constants, R being the experimental value of the ratio for substances A and A′. (Thus for *cis*-1,2-diethoxyethene, 2.3, Σ' contains one term from 2.3.1, while Σ'' contains three terms from 2.3, 2.3.2 and 2.4.2, a total of 4 measurements.) The sum leads to as many linear equations for the parameters as there are different substances by the usual technique of minimizing the sum. The equations are, however, coupled through the terms in the Σ'' sum. The equations may be solved iteratively as uncoupled linear equations by using values from the previous cycle for $\langle k_r^{A'} \rangle$ in:

$$0 = \Sigma'\ln(k_r^A) + \Sigma''[\ln(R) + \ln(\langle k_r^{A'} \rangle)] - \Sigma'\ln(\langle k_r^A \rangle) - \Sigma''\ln(\langle k_r^A \rangle)$$

noting that the same ratio data appears in the determination of the parameters for both substances. The last two terms are just $-n\cdot\ln(\langle k_r^A \rangle)$, where n is the number of measurements involving A. Convergence of the iterative process is rapid to the level of six figure precision.

A qualitative measure of how well the $\langle k_r \rangle$ values represent the data is obtained by a histogram, as in figure 3, of the number of values in each interval of log $(k_r/\langle k_r \rangle)$ ranging from −1.0 to +1.0 which shows two orders of magnitude in the ratio. Any value outside of the range of the plot is included in the appropriate extreme interval. We expect that if the global fitting is appropriate, then the histogram should have an approximately Gaussian shape representing a normal distribution of values for $\log(k_r/\langle k_r \rangle)$. As a comparison a normal curve is superimposed on the histogram that has the same area and the same standard deviation as the data.

The initial fitting includes all of the selected data, 490 measurements. This results in 56 values of $\langle k_r \rangle$ with a standard deviation of 0.430. The value of the standard deviation is reduced by removing the measurements outside of the range $-1.0 < \log(k_r/\langle k_r \rangle) < +1.0$. A small additional reduction in the standard deviation is obtained by readjustment of the values of $\langle k_r \rangle$ to the reduced set of measurements, further the histogram looks a bit more like the normal curve. The value of the standard deviation becomes 0.298 which corresponds to a factor of 1.99 for the ratio of k_r to $\langle k_r \rangle$. This implies that any specific measured value k_r should differ from the adjusted value $\langle k_r \rangle$ by less than a factor of 4 (the 95% confidence level being $10^{2\times0.298} \approx 4$).

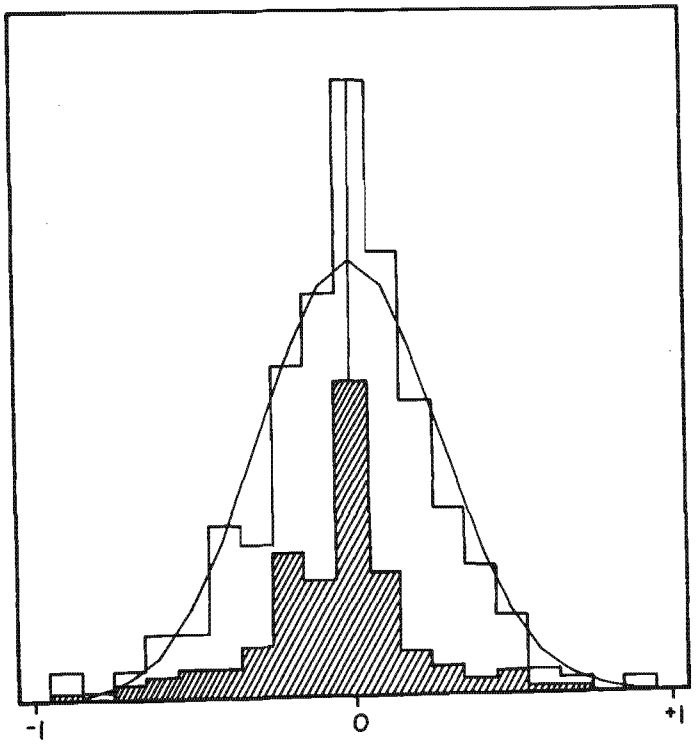

FIGURE 3. Histogram of relative deviations between measured values of k_r and the values $\langle k_r \rangle$ selected to give the least square fit to all of the measured values. The intervals are of size 0.1 in $\log_{10}(k_r/\langle k_r \rangle)$, the full range being from −1.0 to + 1.0 covers a factor of 10 smaller and larger in the rate constants. The filled area represents measurements of ratios of rates. The superimposed curve represents a normal distribution of the same area and standard deviation as the data represented by the histogram.

The values of $\langle k_r \rangle$, the best estimates of the values of the rate constants, corresponding to the histogram figure 3, are tabulated in table A1. Each compound is listed by table number from tables 2 through 15, thus ethoxyethene is listed as 2.1, is associated with the value 7.03×10^4 for $\langle k_r \rangle$, an estimate of the 95% confidence limits of a factor of 2.98 for $\langle k_r \rangle$ and the number of measurements included is 4. The 95% confidence limits are obtained from the standard deviation of the global fit and the number of measurements (N) for a substance, either directly or as a ratio of rates relative to some other substance. The 95% confidence limits of $\log(\langle k_r \rangle)$ are the standard deviation times a factor from Student's t distribution (ranging from 12.7 for 2 measurements to 2.0 for many measurements for the 95% confidence level). This would be an additive range for $\log(\langle k_r \rangle)$, thus for values of $\langle k_r \rangle$ the range would be given as a multiplicative factor, the range for ethoxyethene being from 2.4×10^4 to 2.1×10^5. Substances with only one value reported have no standard deviation and those with only two values are listed as having a factor of > 10.

It may be noted that as reported only compounds with 7 or more measurements claim confidence limits of less than a factor of 2. The uncertainty in values for individual measurements is so great, standard deviation in the logarithm of 0.298, that in only one case is the value of $\langle k_r \rangle$ as narrow as the values of uncertainty in k_r assigned by many of the experimental groups. We list 104 values for diphenylisobenzofuran of having the average value of many measurements determined to better than the expected uncertainty of individual measurements.

One may well ask if these values support the idea that solvent effects are less important than the range of uncertainty in the experimental data. One may argue that the values from a single laboratory are internally more consistent than the values between laboratories, thus showing solvent effects too small to show up in our treatment. Nonetheless it is desirable to examine the present set of data for solvent effects. One approach is to look for an average effect on all compounds, a second approach is to look for changes for each compound in different solvents. Both approaches largely support the independence of k_r from effect by most solvents but not all solvents. The former draws into doubt the solvents H_2O, as leading to increased values of k_r, and CCl_4, as leading to reduced values. The latter approach singles out several substances as having rates significantly different in one solvent, as is indicated in table A2.

Table A2 separately averages all combinations of compound and solvent for which there are at least two measurements and estimates a 95% confidence factor for the average. Generally this results in there being fewer values to average but not always to a large 95% range. As an example the first entry (2.1, ethoxyethene) shows three values reported for acetone as solvent. The best value, assuming no solvent effect is 7.03×10^4, while the average of the three values for acetone as solvent is 4.74×10^4, the ratio of these two values is 1.48 and to be significant to the 95% confidence level the ratio

TABLE A1. Adjusted best values of rate constants, k_r, for reaction of substrates with singlet oxygen

Substrate	$\langle k_r \rangle$[a]/ $dm^3\ mol^{-1}\ s^{-1}$	95%[b]	N[c]
2.1[d]	7.03×10^4	2.98	4
2.3	3.87×10^7	2.98	4
2.4	2.07×10^7	5.49	3
2.12	3.98×10^7	2.34	5
2.33	1.49×10^6	1.35	23
2.35	2.97×10^7	1.26	36
2.40	8.13×10^5	1.27	34
2.42	9.11×10^5	2.34	5
2.43	1.19×10^6	2.98	4
2.45	1.13×10^4	2.98	4
2.50	5.67×10^4	>10.00	2
2.52	1.78×10^6	1.50	14
2.53	2.82×10^4	>10.00	2
2.54	2.98×10^3	5.49	3
2.55	2.89×10^5	2.05	6
2.56	1.98×10^5	1.28	30
2.58	1.16×10^7	2.34	5
2.59	1.90×10^5	>10.00	2
2.64	1.02×10^5	>10.00	2
2.71	1.20×10^5	2.98	4
2.74	2.03×10^4	1.77	8
2.75	4.90×10^4	5.9	3
2.86	3.00×10^7	2.34	5
2.90	2.00×10^6	1.89	7
2.91	3.49×10^6	1.89	7
2.130	1.15×10^{10}	1.45	15
3.10	5.26×10^6	5.49	3
3.12	3.31×10^6	5.49	3
3.13	6.74×10^6	2.34	5
3.18	9.43×10^6	2.98	4
3.53	4.71×10^7	1.28	31
3.56	1.51×10^6	1.69	9
3.61	3.20×10^7	1.77	8
3.62	1.21×10^7	1.77	8
3.63	4.16×10^7	1.27	34
4.7	2.55×10^6	2.98	4
4.9	8.11×10^5	>10.00	2
4.12	1.09×10^6	5.49	3
4.28	1.46×10^6	5.49	3
5.22	4.65×10^6	2.98	4
5.29	2.33×10^8	1.50	14
5.30	6.98×10^7	1.27	34
5.36	6.34×10^8	1.14	104
7.17	8.07×10^9	>10.00	2
9.1	5.89×10^8	1.77	8
9.4	3.46×10^8	2.98	4
9.6	5.56×10^7	2.34	5
11.45	9.78×10^7	>10.00	2
14.5	1.13×10^5	5.49	3
14.6	1.81×10^5	5.49	3
14.7	2.26×10^5	2.98	4
14.9	8.44×10^4	1.89	7
14.32	1.86×10^8	1.69	9

[a]Prefered value of k_r.
[b]95% confidence limits on $\langle k_r \rangle$.
[c]Number of k_r values included in the determination of $\langle k_r \rangle$.
[d]Entry numbers in tables 2–14 where substrates are identified and reported rate data for substrates are given.

TABLE A2. The effect of solvent on k_r, rate constants for reaction of substrates with singlet oxygen

Substrate	Solvent	N[a]	$\langle k_r \rangle$[b]/ $dm^3\ mol^{-1}\ s^{-1}$	Average k_r[c]/ $dm^3\ mol^{-1}\ s^{-1}$	Ratio[d]	95%[e]
2.1[f]	$(Me)_2CO$	3	7.03×10^4	4.74×10^4	1.48	2.74
2.3	$(Me)_2CO$	4	3.87×10^7	3.87×10^7	1.00	1.32
2.4	$(Me)_2CO$	3	2.07×10^7	2.07×10^7	1.00	3.86
2.12	$(Me)_2CO$	2	3.98×10^7	3.02×10^7	1.32	9.31
2.33	MeOH	8	1.49×10^6	1.22×10^6	1.22	2.08
2.33	X[g]	15	1.49×10^6	1.66×10^6	1.11	1.33
2.35	C_5H_5N	5	2.97×10^7	1.84×10^7	1.61	2.10
2.35	$(Me)_2CO$	3	2.97×10^7	4.18×10^7	1.41	1.36*
2.35	MeOH	5	2.97×10^7	2.52×10^7	1.18	1.57
2.35	X	16	2.97×10^7	3.66×10^7	1.23	1.41
2.40	C_5H_5N	2	8.13×10^5	1.30×10^6	1.59	2.66
2.40	C_6H_6	6	8.13×10^5	9.43×10^5	1.16	3.37
2.40	CH_3CN	2	8.13×10^5	1.59×10^6	1.95	4.93
2.40	$(Me)_2SO$	2	8.13×10^5	8.38×10^5	1.03	4.89
2.40	MeOH	8	8.13×10^5	6.24×10^5	1.30	1.14*
2.40	X	7	8.13×10^5	9.04×10^5	1.11	1.22
2.40	Y[g]	2	8.13×10^5	7.63×10^5	1.07	1.00*
2.42	X	4	9.11×10^5	8.34×10^5	1.09	1.56
2.43	X	4	1.19×10^6	3.58×10^5	3.32	49.98
2.45	X	4	1.13×10^4	1.13×10^4	1.00	1.50
2.50	MeOH	2	5.67×10^4	5.67×10^4	1.00	4.03
2.52	C_6H_6	4	1.78×10^6	2.32×10^6	1.31	1.09*
2.52	MeOH	6	1.78×10^6	1.86×10^6	1.05	1.17
2.52	X	3	1.78×10^6	1.19×10^6	1.49	1.80
2.53	MeOH	2	2.82×10^4	2.82×10^4	1.00	4.03
2.54	MeOH	2	2.98×10^3	3.55×10^3	1.19	2.35
2.55	$(Me)_2CO$	6	2.89×10^5	2.89×10^5	1.00	1.55
2.56	C_6H_6	4	1.98×10^5	2.97×10^5	1.50	1.14*
2.56	CH_3CN	6	1.98×10^5	2.43×10^5	1.23	2.12
2.56	$(Me)_2CO$	2	1.98×10^5	4.17×10^5	2.10	>100.00
2.56	MeOH	8	1.98×10^5	1.46×10^5	1.35	1.41
2.56	X	9	1.98×10^5	2.38×10^5	1.20	4.12
2.58	MeOH	4	1.16×10^7	9.10×10^6	1.27	3.05
2.59	MeOH	2	1.90×10^5	1.90×10^5	1.00	4.03
2.64	CH_3CN	2	1.02×10^5	1.02×10^5	1.00	>100.00
2.71	CH_3CN	4	1.20×10^5	1.20×10^5	1.00	4.29
2.74	CH_3CN	2	2.03×10^4	2.14×10^4	1.06	>100.00
2.74	MeOH	6	2.03×10^4	1.99×10^4	1.02	1.52
2.75	CH_3CN	2	4.90×10^4	3.43×10^4	1.43	3.22
2.86	MeOH	2	3.00×10^7	2.35×10^7	1.28	1.30
2.86	X	3	3.00×10^7	3.53×10^7	1.18	3.68
2.90	MeOH	2	2.00×10^6	3.33×10^6	1.66	>100.00
2.90	X	2	2.00×10^6	3.84×10^6	1.92	>100.00
2.91	MeOH	5	3.49×10^6	3.09×10^6	1.13	2.42
2.91	X	2	3.49×10^6	4.75×10^6	1.36	>100.00

TABLE A2. The effect of solvent on k_r, rate constants for reaction of substrates with singlet oxygen — Continued

Substrate	Solvent	N[a]	$\langle k_r \rangle$[b]/ $dm^3\ mol^{-1}\ s^{-1}$	Average k_r[c]/ $dm^3\ mol^{-1}\ s^{-1}$	Ratio[d]	95%[e]
2.130	C_6H_6	5	1.15×10^{10}	2.66×10^{9}	4.32	96.40
2.130	Y	6	1.15×10^{10}	9.67×10^{9}	1.19	2.83
3.10	X	2	5.26×10^{6}	5.50×10^{6}	1.05	1.32
3.12	MeOH	2	3.31×10^{6}	3.20×10^{6}	1.03	1.62
3.13	X	2	6.74×10^{6}	6.30×10^{6}	1.07	1.00*
3.13	Y	2	6.74×10^{6}	6.96×10^{6}	1.03	1.26
3.18	Y	3	9.43×10^{6}	9.51×10^{6}	1.01	1.20
3.53	C_5H_5N	5	4.71×10^{7}	4.85×10^{7}	1.03	1.21
3.53	C_6H_6	8	4.71×10^{7}	6.96×10^{7}	1.48	1.85
3.53	CH_3CN	4	4.71×10^{7}	8.08×10^{7}	1.72	2.48
3.53	$CHCl_3$	5	4.71×10^{7}	6.12×10^{7}	1.30	1.95
3.53	EtOH	3	4.71×10^{7}	2.74×10^{7}	1.72	5.95
3.53	H_2O	2	4.71×10^{7}	8.26×10^{8}	17.55	3.41*
3.53	MeOH	2	4.71×10^{7}	2.03×10^{7}	2.32	>100.00
3.56	C_6H_6	4	1.51×10^{6}	8.04×10^{5}	1.87	1.36*
3.61	C_6H_6	8	3.20×10^{7}	3.20×10^{7}	1.00	1.64
3.62	C_6H_6	5	1.21×10^{7}	1.44×10^{7}	1.19	1.62
3.62	CCl_4	2	1.21×10^{7}	5.00×10^{6}	2.42	1.00*
3.63	C_5H_5N	3	4.16×10^{7}	5.06×10^{7}	1.22	3.34
3.63	C_6H_6	13	4.16×10^{7}	5.08×10^{7}	1.22	1.31
3.63	CCl_4	5	4.16×10^{7}	3.66×10^{7}	1.14	2.48
3.63	$CHCl_3$	4	4.16×10^{7}	3.76×10^{7}	1.11	2.09
3.63	CS_2	3	4.16×10^{7}	5.09×10^{7}	1.22	5.26
4.7	C_6H_6	4	2.55×10^{6}	9.66×10^{6}	3.78	>100.00
4.7	MeOH	2	2.55×10^{6}	4.84×10^{6}	1.90	6.32
4.12	C_6H_6	2	1.09×10^{6}	6.20×10^{5}	1.77	>100.00
5.22	MeOH	2	4.65×10^{6}	2.89×10^{7}	6.21	7.85
5.29	EtOH	5	2.33×10^{8}	2.09×10^{8}	1.11	4.97
5.29	H_2O	4	2.33×10^{8}	1.13×10^{9}	4.86	2.38*
5.29	MeOH	5	2.33×10^{8}	2.89×10^{8}	1.24	2.09
5.29	X	4	2.33×10^{8}	1.24×10^{8}	1.87	5.30
5.30	$C_6H_{11}OH$	2	6.98×10^{7}	5.25×10^{7}	1.33	1.14*
5.30	CH_2Cl_2	2	6.98×10^{7}	8.64×10^{7}	1.24	1.06*
5.30	CH_3CN	2	6.98×10^{7}	1.51×10^{8}	2.16	37.05
5.30	*i*-PrOH	2	6.98×10^{7}	4.88×10^{7}	1.43	1.23*
5.30	$(Me)_2CO$	2	6.98×10^{7}	1.10×10^{8}	1.58	>100.00
5.30	MeOH	7	6.98×10^{7}	3.69×10^{7}	1.89	2.84
5.30	*n*-BuOH	4	6.98×10^{7}	8.72×10^{7}	1.25	4.59
5.30	*t*-BuOH	4	6.98×10^{7}	9.52×10^{7}	1.36	7.93
5.36	C_5H_5N	5	6.34×10^{8}	9.03×10^{8}	1.42	2.06
5.36	$C_6H_{11}OH$	3	6.34×10^{8}	2.93×10^{8}	2.17	10.53
5.36	C_6H_5Br	2	6.34×10^{8}	5.64×10^{8}	1.12	1.74
5.36	C_6H_6	9	6.34×10^{8}	6.90×10^{8}	1.09	1.40
5.36	CCl_4	3	6.34×10^{8}	2.84×10^{8}	2.23	11.84
5.36	CH_2Cl_2	4	6.34×10^{8}	8.58×10^{8}	1.35	1.84
5.36	CH_3CN	3	6.34×10^{8}	1.36×10^{9}	2.15	73.30
5.36	$CHCl_3$	5	6.34×10^{8}	4.91×10^{8}	1.29	2.10
5.36	dioxane	3	6.34×10^{8}	9.32×10^{8}	1.47	1.76
5.36	EtOH	3	6.34×10^{8}	8.31×10^{8}	1.31	4.05
5.36	H_2O	5	6.34×10^{8}	8.87×10^{9}	13.98	3.23*
5.36	*i*-PrOH	3	6.34×10^{8}	3.92×10^{8}	1.62	9.36
5.36	$(Me)_2CO$	3	6.34×10^{8}	6.21×10^{8}	1.02	1.25
5.36	$C_6H_5CH_3$	2	6.34×10^{8}	3.43×10^{8}	1.85	13.14
5.36	MeOH	14	6.34×10^{8}	1.03×10^{9}	1.63	1.28*
5.36	*n*-BuOH	4	6.34×10^{8}	7.73×10^{8}	1.22	1.76
5.36	*t*-BuOH	4	6.34×10^{8}	5.04×10^{8}	1.26	3.01
5.36	THF	2	6.34×10^{8}	6.23×10^{8}	1.02	16.19
5.36	Y	29	6.34×10^{8}	5.53×10^{8}	1.15	1.39
7.17	EtOH	2	8.07×10^{9}	8.07×10^{9}	1.00	53.62

TABLE A2. The effect of solvent on k_r, rate constants for reaction of substrates with singlet oxygen — Continued

Substrate	Solvent	N[a]	$\langle k_r \rangle$[b]/ $dm^3\ mol^{-1}\ s^{-1}$	Average k_r[c]/ $dm^3\ mol^{-1}\ s^{-1}$	Ratio[d]	95%[e]
9.1	CH_3CN	4	5.89×10^8	6.46×10^8	1.10	2.01
9.1	$CHCl_3$	2	5.89×10^8	5.36×10^8	1.10	2.41
9.1	MeOH	2	5.89×10^8	5.36×10^8	1.10	4.10
9.4	CH_3CN	3	3.46×10^8	3.48×10^8	1.01	4.42
9.6	$CHCl_3$	4	5.56×10^7	3.85×10^7	1.44	2.11
11.45	C_6H_6	2	9.78×10^7	9.78×10^7	1.00	1.32
14.5	C_5H_5N	2	1.13×10^5	1.05×10^5	1.07	4.63
14.6	C_5H_5N	2	1.81×10^5	1.65×10^5	1.10	1.38
14.6	EtOH	2	1.81×10^5	5.40×10^6	29.78	>100.00
14.7	C_5H_5N	3	2.26×10^5	2.07×10^5	1.09	1.76
14.9	C_5H_5N	7	8.44×10^4	8.44×10^4	1.00	1.14
14.32	CCl_4	2	1.86×10^8	1.66×10^8	1.12	1.00*
14.32	$CHCl_3$	3	1.86×10^8	2.27×10^8	1.22	1.52
14.32	D_2O	2	1.86×10^8	1.33×10^8	1.40	>100.00
14.32	Y	2	1.86×10^8	1.58×10^8	1.18	>100.00

[a]Number of k_r values determined in this particular solvent.
[b]Preferred value of k_r.
[c]Average value of k_r for this particular solvent.
[d]Ratio of Average value of k_r for this particular solvent to $\langle k_r \rangle$; ratio is inverted if less than one.
[e]95% confidence limits on Ratio. Only values marked with an asterisk are less than the Ratio.
[f]Entry number in tables 2–14 where substrates are identified and reported rate data for substrates are given.
[g]Solvent X = MeOH/*t*-BuOH (1:1); solvent Y = other mixed solvents.

TABLE A3. Preferred values of k_r, rate constants for reaction of substrates with singlet oxygen

No.[a]	Substrate	$<k_r>$[b]/ $dm^3\ mol^{-1}\ s^{-1}$	95%[c]
A3.1	2-methyl-2-butene (2M2B, 2.33)[e]	1.49×10^6	1.35
A3.2	2,3-dimethyl-2-butene (TME, 2.35)	2.97×10^7	1.26
A3.3	2-methyl-2-pentene (2M2P, 2.40)	8.13×10^5	1.27
A3.4	1-methylcyclopentene (2.52)	1.78×10^6	1.50
A3.5	1-methylcyclohexene (2.56)	1.98×10^5	1.28
A3.6	α-pinene (2.74)	2.03×10^4	1.77
A3.7	2,5-dimethyl-2,4-hexadiene (2.90)	2.00×10^6	1.89
A3.8	1,3-cyclohexadiene (2.91)	3.49×10^6	1.89
A3.9	β-carotene (Car, 2.130)	1.15×10^{10}	1.45
A3.10	9,10-dimethylanthracene (DMA, 3.53)	4.71×10^7	1.28
A3.11	9,10-diphenylanthracene (3.56)	1.51×10^6	1.69
A3.12	9,10-dimethyl-1,2-benzanthracene (DMBA, 3.61)	3.20×10^7	1.77
A3.13	2,3-benzanthracene (3.62)	1.21×10^7	1.77
A3.14	β-rubrene (Rub, 3.63)	4.16×10^7	1.27
A3.15	2,5-dimethylfuran (5.29)	2.33×10^8	1.50
A3.16	2,5-diphenylfuran (DPF, 5.30)	6.98×10^7	1.27
		β(MeOH) = 1.4×10^{-3} [d]	
A3.17	1,3-diphenylisobenzofuran (DPBF, 5.36)	6.34×10^8	1.14
A3.18	diazodiphenylmethane (DDM, 9.1)	5.89×10^8	1.77
A3.19	cholesterol (14.9)	8.44×10^4	1.89
A3.20	*bilirubin* (14.32)	1.86×10^8	1.69

[a]Entry numbers used in the Comments column in tables 1–15 to index preferred values of k_r.
[b]Preferred value of k_r.
[c]95% confidence limits on $\langle k_r \rangle$.
[d]β(MeOH) for 2,5-diphenylfuran is calculated by taking the ratio of k_d = *$1.0 \times 10^5\ s^{-1}$ [*1.3.6*] to $\langle k \rangle_r = 6.98 \times 10^7\ dm^3\ mol^{-1}\ s^{-1}$ [*A3.16*].
[e]Entry number in tables 2–15 where reported rate data for substrates are given, and abbreviation in comments column when used as a reference substrate.

should exceed 2.75. Table entries for which the ratio exceeds the statistical 95% confidence level are marked with an asterisk. Several of these represent repeated values by one group of workers and thus may show less variation (and thus smaller statistical confidence limits) than would be the case if several different groups were reporting values. This is the case for 2.52, 1-methylcyclopentene, in benzene. This table seems to support the supposition that as a solvent H_2O is associated with values of k_r that are a factor of 3 or more larger than is the case for other solvents, and perhaps CCl_4 is associated with rates being smaller by a factor of 2. On this basis measurements with H_2O as a solvent have been excluded from the final fitting of $\langle k_r \rangle$ values.

The fitting process itself seems to be internally consistent in that the histogram shows fairly good agreement with the normal distribution of values and there seems to be little correlation with solvent beyond that to be expected from the general variation of reported rate constants. The wide limits of variation of individual measurements, a factor of 2, leads to uncertainty in any results which are larger than we would wish. Nonetheless the values obtained from the fitting are probably the most justifiable values we could choose from these data. For most compounds there are only a few measurements in any solvent, and justification for using those values in other solvents is of value. For the special cases of water or carbon tetrachloride as solvents one may well wish to use other values.

In several of the tables values of k_r have been calculated from measured ratios by multiplying the ratio with a preferred value for the rate of the reference compound. The preferred value was chosen to be $\langle k_r \rangle$ from table A1 when the indicated 95% confidence limits are less than 2.0, that is where there are 7 or more reported values. These values are listed in table A3 as preferred values of these selected rate constants.